



Full wwPDB EM Validation Report ⓘ

Sep 23, 2026 – 05:13 pm BST

PDB ID : 9IF7 / pdb_00009if7
EMDB ID : EMD-52843
Title : Cryo-EM structure of the kinetoplastid trans-spliceosome activated for catalytic step II (C* complex)
Authors : Nadenoen, T.; Vanden Broeck, A.
Deposited on : 2025-02-17
Resolution : 2.70 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

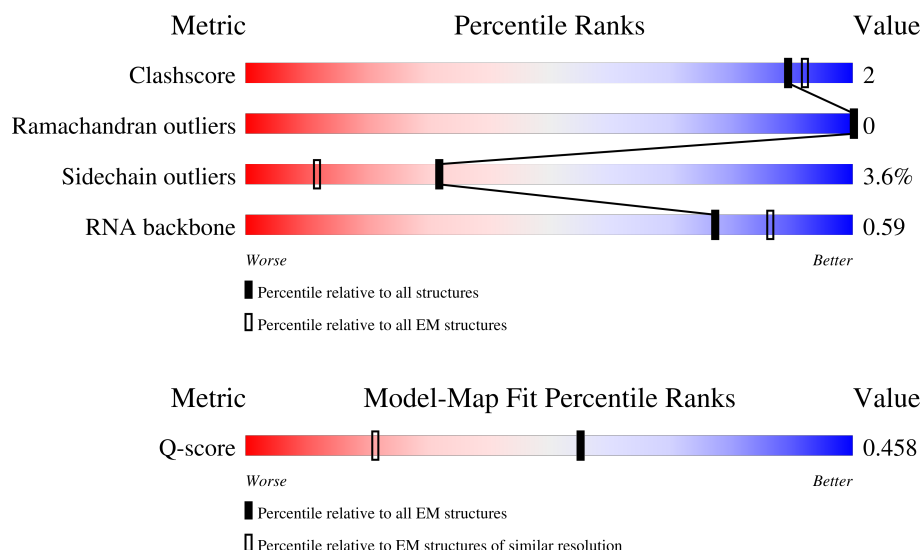
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10327 (2.20 - 3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	L7	389	 5% 88% 11%
2	L8	153	 5% 78% 18%
3	L9	162	 6% 88% 6% 6%

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Mol	Chain	Length	Quality of chain
4	LA	2427	
5	LB	2367	
6	LC	1016	
7	LD	166	
8	LF	706	
9	LG	82	
10	LH	159	
11	LJ	509	
12	LL	326	
13	LN	322	
14	LP	207	
15	LQ	804	
16	LR	197	
17	LS	824	
18	LT	794	
19	LV	1087	
20	LW	307	
21	LY	114	
22	LZ	403	
23	SA	564	
24	SC	417	
25	SD	546	
26	SF	258	
27	SJ	414	
28	SK	175	

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Mol	Chain	Length	Quality of chain
29	SL	544	
30	SN	192	
31	SO	621	
32	SP	269	
33	SQ	150	
34	SS	284	
35	ST	513	
35	SU	513	
35	SV	513	
35	SW	513	
36	TN	1181	
37	UX	21	
38	62	190	
39	63	134	
40	64	116	
41	65	151	
42	66	80	
43	67	91	
44	68	131	
45	RN	68	
46	24	102	
46	51	102	
46	U1	102	
47	25	103	
47	52	103	

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Mol	Chain	Length	Quality of chain
47	U2	103	
48	2C	128	
49	2D	141	
50	2H	86	
50	5E	86	
50	UE	86	
51	2I	76	
51	5F	76	
51	UF	76	
52	2J	81	
52	5G	81	
52	UG	81	
53	53	113	
53	U3	113	
54	5B	111	
54	UB	111	
55	LE	39	
56	LO	57	
57	N2	142	
58	N5	71	
59	N6	100	

2 Entry composition

There are 67 unique types of molecules in this entry. The entry contains 135855 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Probable eukaryotic initiation factor 4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L7	382	Total	C	N	O	S	0	0
			3021	1906	536	558	21		

- Molecule 2 is a protein called RRM domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L8	125	Total	C	N	O	S	0	0
			999	634	165	198	2		

- Molecule 3 is a protein called Mago nashi-like protein,putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L9	152	Total	C	N	O	S	0	0
			1243	795	211	233	4		

- Molecule 4 is a protein called Prp8 protein homologue, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	LA	2347	Total	C	N	O	S	2	0
			18216	11549	3257	3315	95		

- Molecule 5 is a protein called ATP-dependent RNA helicase, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	LB	2128	Total	C	N	O	0	0
			10536	6280	2128	2128		

- Molecule 6 is a protein called Small nuclear ribonucleoprotein component-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	LC	911	Total	C	N	O	S	0	0
			7002	4420	1231	1323	28		

- Molecule 7 is a protein called PRKR-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LD	125	Total	C	N	O	S	0	0
			1006	603	215	187	1		

- Molecule 8 is a protein called Splicing factor Cactin C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LF	408	Total	C	N	O	S	0	0
			3311	2102	598	594	17		

- Molecule 9 is a protein called RNA-binding motif protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LG	80	Total	C	N	O	S	0	0
			592	372	101	115	4		

- Molecule 10 is a protein called Splicing regulator SDE2-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LH	42	Total	C	N	O	S	0	0
			331	208	68	54	1		

- Molecule 11 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LJ	413	Total	C	N	O	S	0	0
			3196	2015	575	590	16		

- Molecule 12 is a protein called G10 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LL	185	Total	C	N	O	S	1	0
			1455	910	275	254	16		

- Molecule 13 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LN	316	Total	C	N	O	S	0	0
			2314	1430	418	448	18		

- Molecule 14 is a protein called Spliceosome-associated CWC15-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LP	72	Total	C	N	O	S	1	0
			598	378	114	104	2		

- Molecule 15 is a protein called Cell division control protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LQ	551	Total	C	N	O	S	0	0
			4277	2620	824	817	16		

- Molecule 16 is a protein called CWF21 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LR	161	Total	C	N	O	S	0	0
			1230	746	243	236	5		

- Molecule 17 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LS	772	Total	C	N	O	S	0	0
			6209	3867	1170	1149	23		

- Molecule 18 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LT	794	Total	C	N	O	S	0	0
			6284	3978	1133	1142	31		

- Molecule 19 is a protein called RNA helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LV	973	Total	C	N	O	S	0	0
			7589	4749	1326	1465	49		

- Molecule 20 is a protein called U2 small nuclear ribonucleoprotein 40K, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LW	188	Total	C	N	O	S	0	0
			1545	979	280	280	6		

- Molecule 21 is a protein called RRM domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LY	107	Total	C	N	O	S	0	0
			876	558	163	151	4		

- Molecule 22 is a protein called NF-kappa-B-activating protein C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LZ	89	Total	C	N	O	S	0	0
			619	376	123	118	2		

- Molecule 23 is a protein called MI domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	SA	511	Total	C	N	O	S	0	0
			4239	2656	764	793	26		

- Molecule 24 is a protein called Pre-mRNA-splicing factor SLU7.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	SC	261	Total	C	N	O	S	0	0
			2108	1298	389	414	7		

- Molecule 25 is a protein called Pre-mRNA-splicing factor 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	SD	322	Total	C	N	O	S	0	0
			2577	1630	464	468	15		

- Molecule 26 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	SF	48	Total	C	N	O	0	0
			237	141	48	48		

- Molecule 27 is a protein called PRP19-related complex protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	SJ	273	Total	C	N	O	S	0	0
			2197	1359	412	417	9		

- Molecule 28 is a protein called Unspecified product.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	SK	87	Total	C	N	O	S	0	0
			699	452	118	125	4		

- Molecule 29 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	SL	239	Total	C	N	O	P S	0	0
			1770	1074	324	362	1 9		

- Molecule 30 is a protein called peptidylprolyl isomerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	SN	185	Total	C	N	O	S	0	0
			1396	885	239	264	8		

- Molecule 31 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	SO	424	Total	C	N	O	S	0	0
			3334	2111	598	611	14		

- Molecule 32 is a protein called Pre-mRNA-splicing factor ISY1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	SP	83	Total	C	N	O	S	0	0
			683	423	127	132	1		

- Molecule 33 is a protein called Zinc knuckle.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	SQ	106	Total	C	N	O	S	0	0
			838	523	154	156	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SQ	0	ACE	-	acetylation	UNP A0A640KSY0

- Molecule 34 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	SS	186	Total	C	N	O	S	0	0
			1504	936	279	282	7		

- Molecule 35 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	ST	488	Total	C	N	O	S	0	0
			3606	2238	650	700	18		
35	SU	133	Total	C	N	O	S	0	0
			1022	637	184	195	6		
35	SV	133	Total	C	N	O	S	0	0
			1022	637	184	195	6		
35	SW	121	Total	C	N	O	S	0	0
			949	593	172	178	6		

- Molecule 36 is a protein called Probable RNA helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	TN	44	Total	C	N	O	S	0	0
			351	227	59	63	2		

- Molecule 37 is a protein called Unidentified protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	UX	21	Total	C	N	O	0	0
			105	63	21	21		

- Molecule 38 is a protein called LSM domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	62	124	Total	C	N	O	S	0	0
			937	578	177	175	7		

- Molecule 39 is a protein called Sm domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	63	79	Total	C	N	O	S	0	0
			602	377	102	119	4		

- Molecule 40 is a protein called U6 snRNA-associated Sm-like protein LSm4.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	64	83	Total	C	N	O	S	0	0
			640	390	123	121	6		

- Molecule 41 is a protein called LSM domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	65	114	Total	C	N	O	S	0	0
			876	547	151	172	6		

- Molecule 42 is a protein called Sm domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	66	71	Total	C	N	O	S	0	0
			541	338	94	106	3		

- Molecule 43 is a protein called Lsm7p protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	67	91	Total	C	N	O	S	0	0
			701	444	129	126	2		

- Molecule 44 is a protein called Sm domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	68	102	Total	C	N	O	S	0	0
			774	486	136	147	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
68	0	ACE	-	acetylation	UNP A0A640KIZ1

- Molecule 45 is a RNA chain called Y-branched pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	RN	21	Total	C	N	O	P	0	0
			283	120	15	127	21		

- Molecule 46 is a protein called Small nuclear ribonucleoprotein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	24	102	Total	C	N	O	S	0	0
			783	489	132	157	5		
46	51	98	Total	C	N	O	S	0	0
			758	475	127	151	5		
46	U1	98	Total	C	N	O		0	0
			484	288	98	98			

- Molecule 47 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	25	82	Total	C	N	O	S	0	0
			654	418	116	118	2		
47	52	89	Total	C	N	O	S	0	0
			715	457	128	128	2		
47	U2	83	Total	C	N	O		0	0
			411	245	83	83			

- Molecule 48 is a protein called Lsm5p, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	2C	114	Total	C	N	O	S	0	0
			881	535	174	168	4		

- Molecule 49 is a protein called Small nuclear ribonucleoprotein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	2D	99	Total	C	N	O	S	0	0
			792	502	140	148	2		

- Molecule 50 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	2H	81	Total	C	N	O	S	0	0
			657	409	124	120	4		
50	5E	78	Total	C	N	O	S	0	0
			629	393	117	116	3		
50	UE	79	Total	C	N	O		0	0
			388	230	79	79			

- Molecule 51 is a protein called Sm protein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	2I	76	Total	C	N	O	S	0	0
			598	377	104	113	4		
51	5F	76	Total	C	N	O	S	0	0
			598	377	104	113	4		
51	UF	76	Total	C	N	O		0	0
			375	223	76	76			

- Molecule 52 is a protein called Sm protein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	2J	77	Total	C	N	O	S	0	0
			583	361	107	112	3		
52	5G	77	Total	C	N	O	S	0	0
			583	361	107	112	3		
52	UG	77	Total	C	N	O		0	0
			379	225	77	77			

- Molecule 53 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	53	104	Total	C	N	O	S	0	0
			801	502	147	150	2		
53	U3	81	Total	C	N	O		0	0
			400	238	81	81			

- Molecule 54 is a protein called Sm protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	5B	99	Total	C	N	O	S	0	0
			738	458	133	141	6		
54	UB	81	Total	C	N	O		0	0
			398	236	81	81			

- Molecule 55 is a RNA chain called SL RNA exon.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	LE	25	Total	C	N	O	P	1	0
			547	245	88	188	26		

- Molecule 56 is a RNA chain called SL RNA outtron.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	LO	47	Total	C	N	O	P	0	0
			1006	449	183	327	47		

- Molecule 57 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	N2	76	Total	C	N	O	P	0	0
			1604	718	270	540	76		

- Molecule 58 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	N5	63	Total	C	N	O	P	0	0
			1328	595	230	440	63		

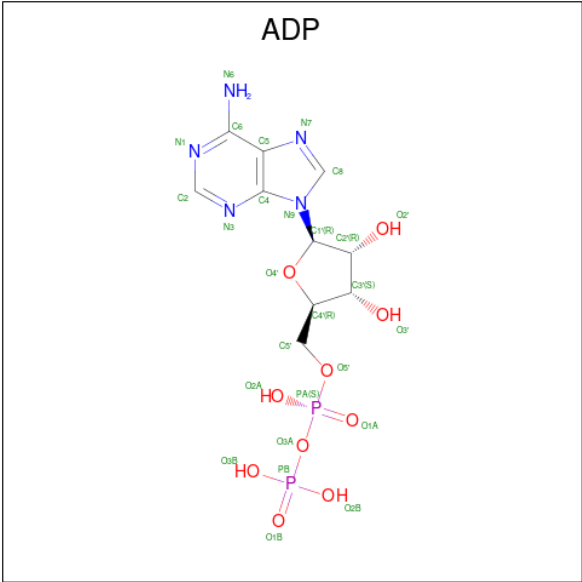
- Molecule 59 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	N6	100	Total	C	N	O	P	0	0
			2127	952	381	694	100		

- Molecule 60 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
60	L7	1	Total	Mg	0
			1	1	
60	LA	1	Total	Mg	0
			1	1	
60	LC	1	Total	Mg	0
			1	1	
60	N5	1	Total	Mg	0
			1	1	
60	N6	8	Total	Mg	0
			8	8	

- Molecule 61 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

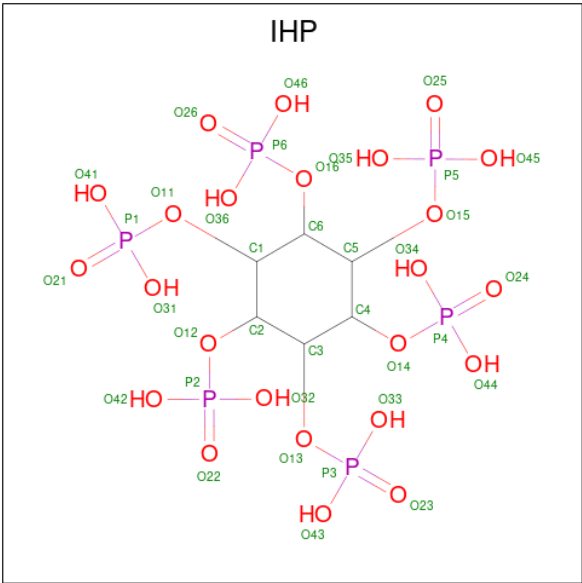


Mol	Chain	Residues	Atoms					AltConf
61	L7	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 62 is POTASSIUM ION (CCD ID: K) (formula: K).

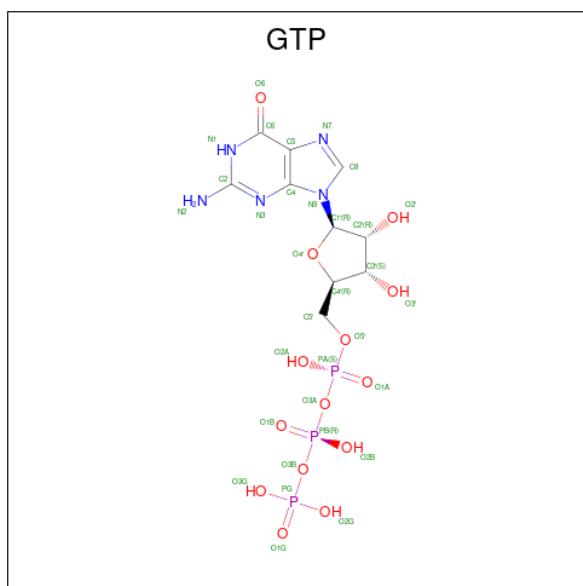
Mol	Chain	Residues	Atoms		AltConf
62	L7	1	Total	K	0
			1	1	

- Molecule 63 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: C₆H₁₈O₂₄P₆).



Mol	Chain	Residues	Atoms				AltConf
63	LA	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 64 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

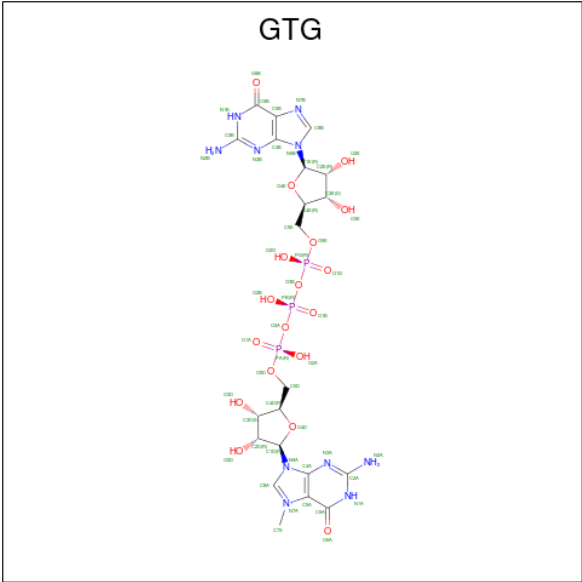


Mol	Chain	Residues	Atoms					AltConf
64	LC	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 65 is ZINC ION (CCD ID: ZN) (formula: Zn).

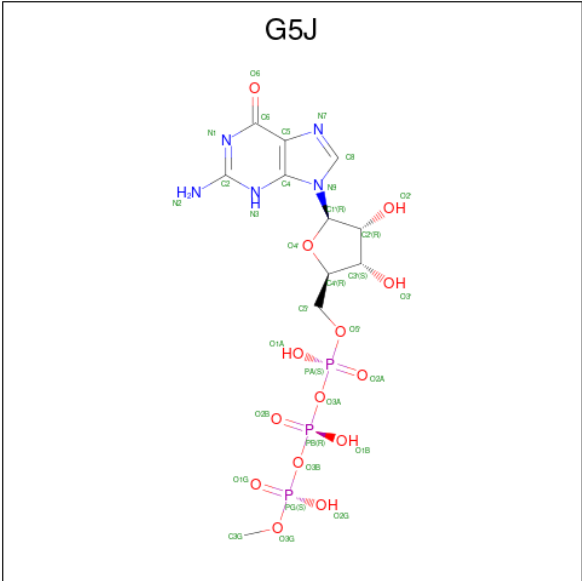
Mol	Chain	Residues	Atoms		AltConf
65	LL	3	Total	Zn	0
			3	3	
65	SC	1	Total	Zn	0
			1	1	
65	SQ	1	Total	Zn	0
			1	1	

- Molecule 66 is 7-METHYL-GUANOSINE-5'-TRIPHOSPHATE-5'-GUANOSINE (CCD ID: GTG) (formula: $C_{21}H_{30}N_{10}O_{18}P_3$).



Mol	Chain	Residues	Atoms					AltConf
66	N5	1	Total	C	N	O	P	0
			52	21	10	18	3	

- Molecule 67 is 5'-O-[(S)-hydroxy{[(R)-hydroxy{[(S)-hydroxy(methoxy)phosphoryl]oxy}phosphoryl]oxy}phosphoryl]guanosine (CCD ID: G5J) (formula: C₁₁H₁₈N₅O₁₄P₃).

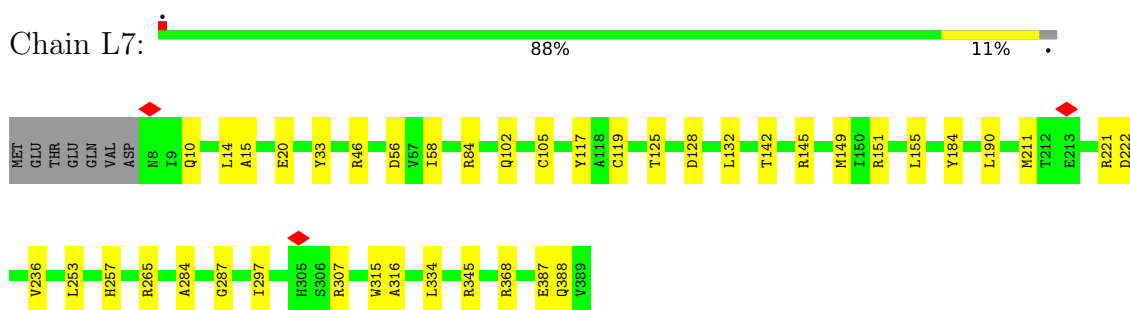


Mol	Chain	Residues	Atoms					AltConf
67	N6	1	Total	C	N	O	P	0
			33	11	5	14	3	

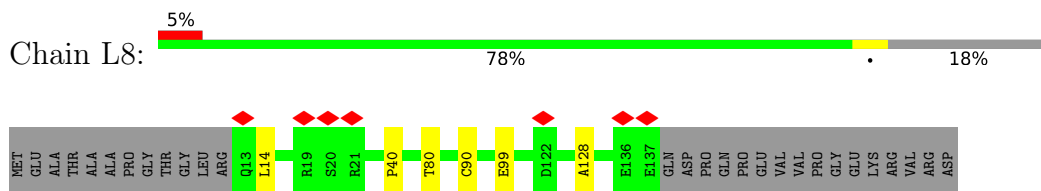
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

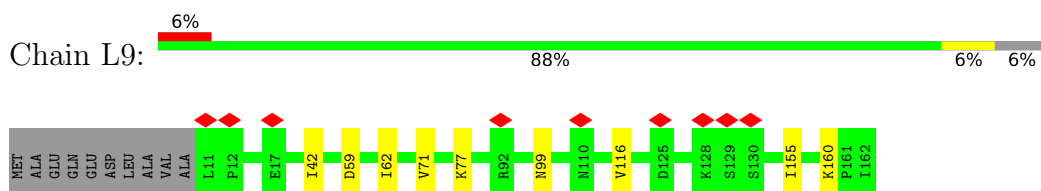
- Molecule 1: Probable eukaryotic initiation factor 4A



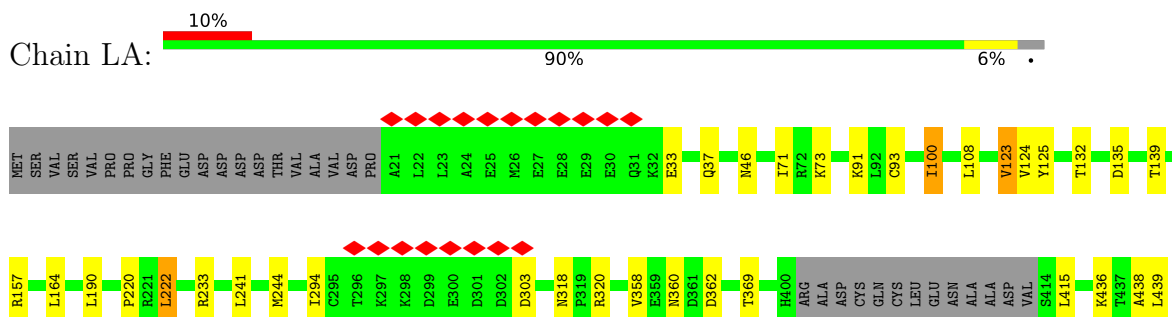
- Molecule 2: RRM domain-containing protein

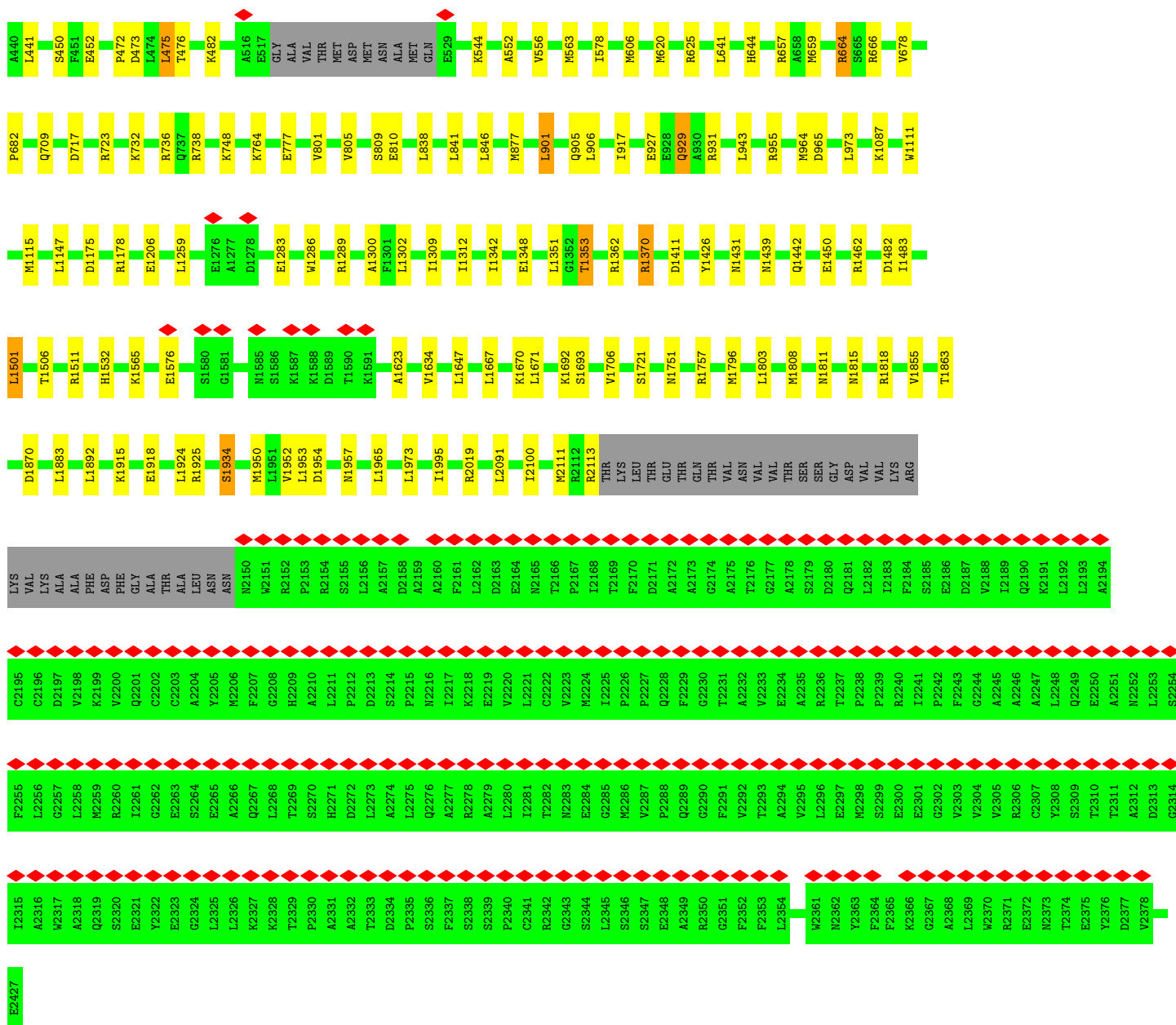


- Molecule 3: Mago nashi-like protein, putative

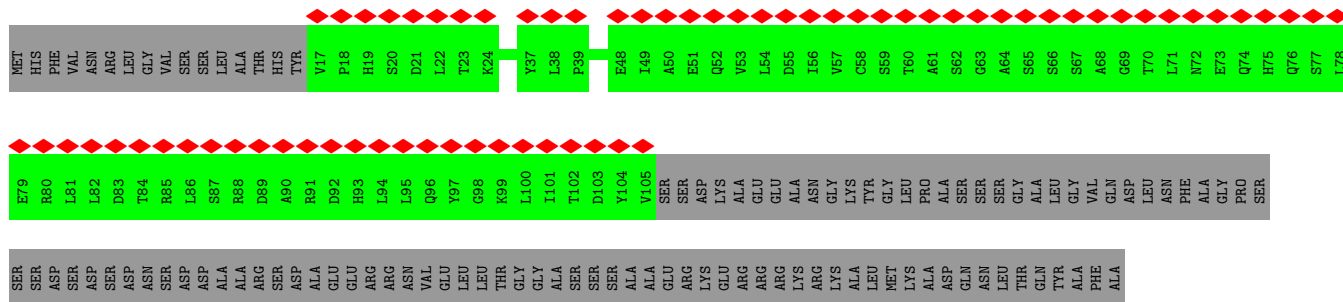
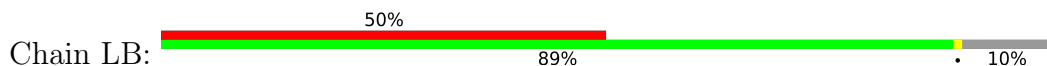


- Molecule 4: Prp8 protein homologue, putative

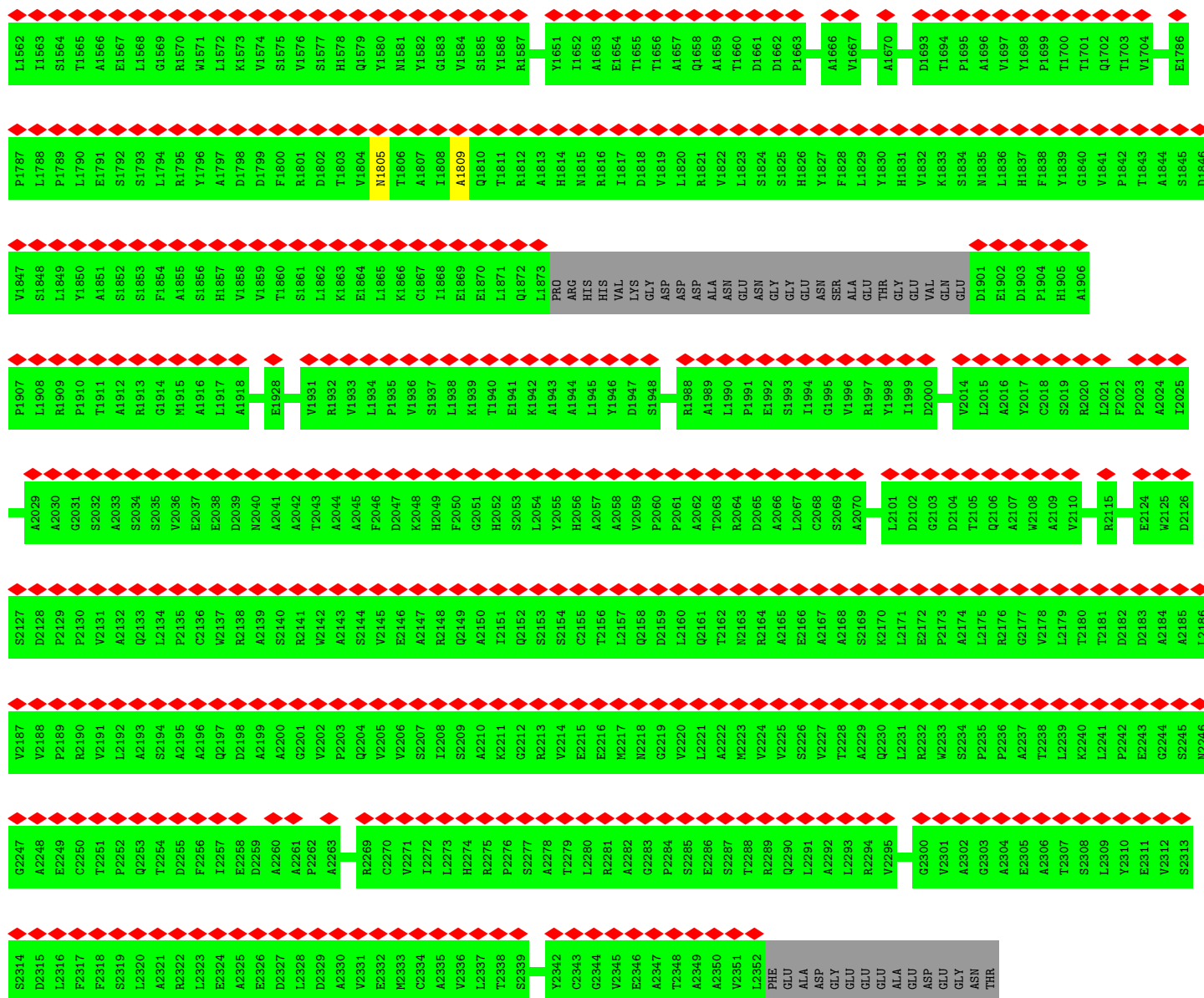




• Molecule 5: ATP-dependent RNA helicase, putative

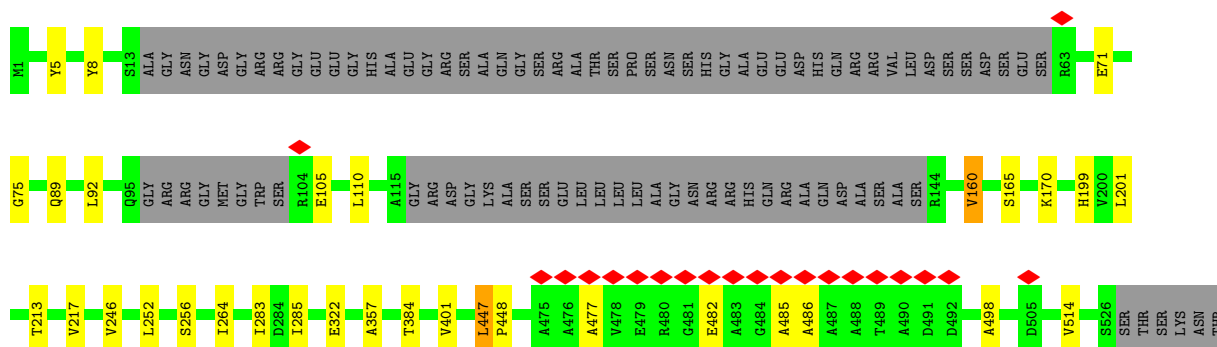


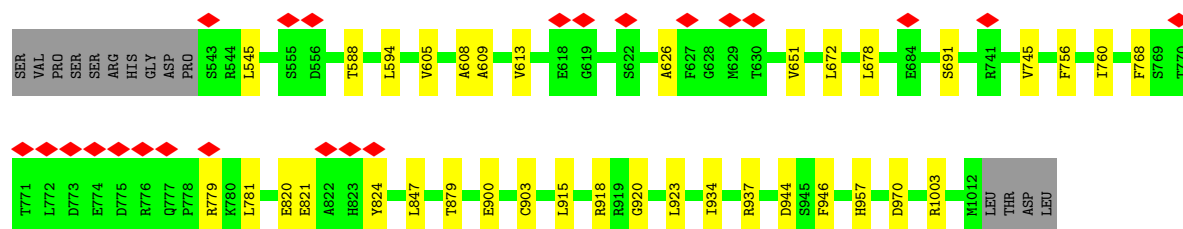




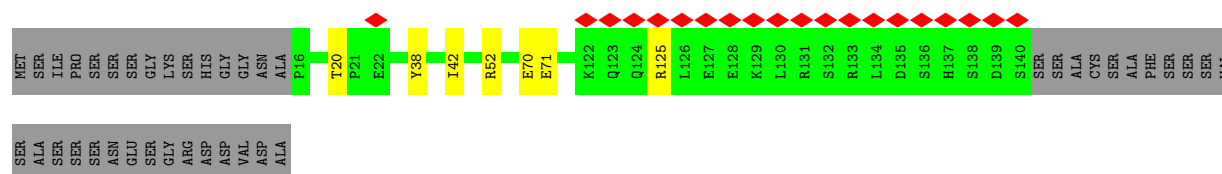
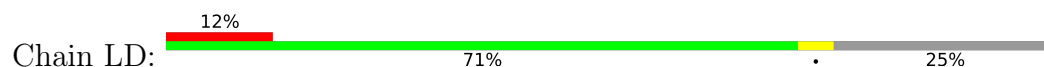
- Molecule 6: Small nuclear ribonucleoprotein component-like protein

Chain LC: 83% 7% 10%

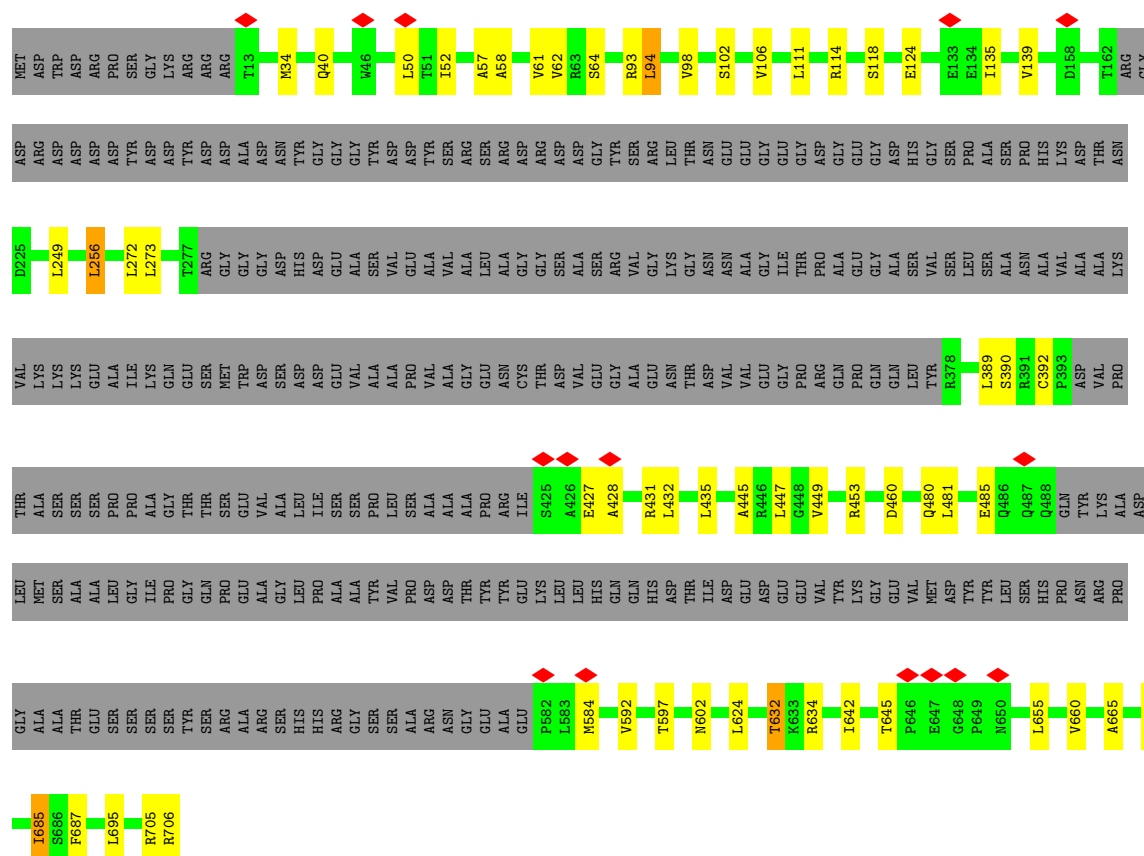




• Molecule 7: PRKR-interacting protein 1



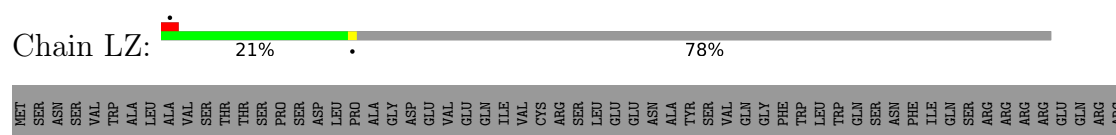
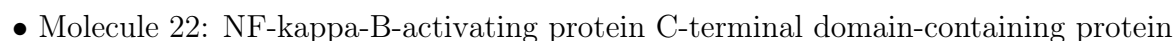
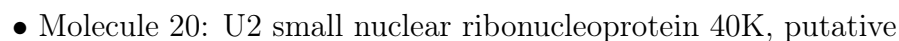
• Molecule 8: Splicing factor Cactin C-terminal domain-containing protein



• Molecule 9: RNA-binding motif protein

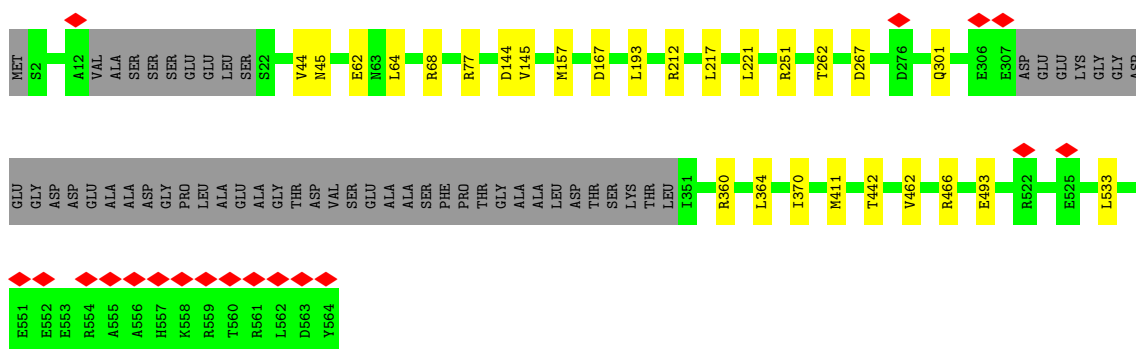




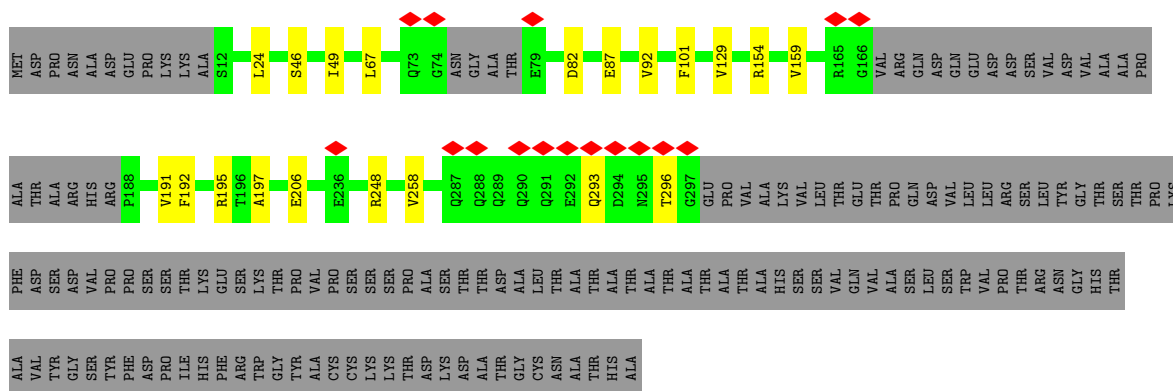




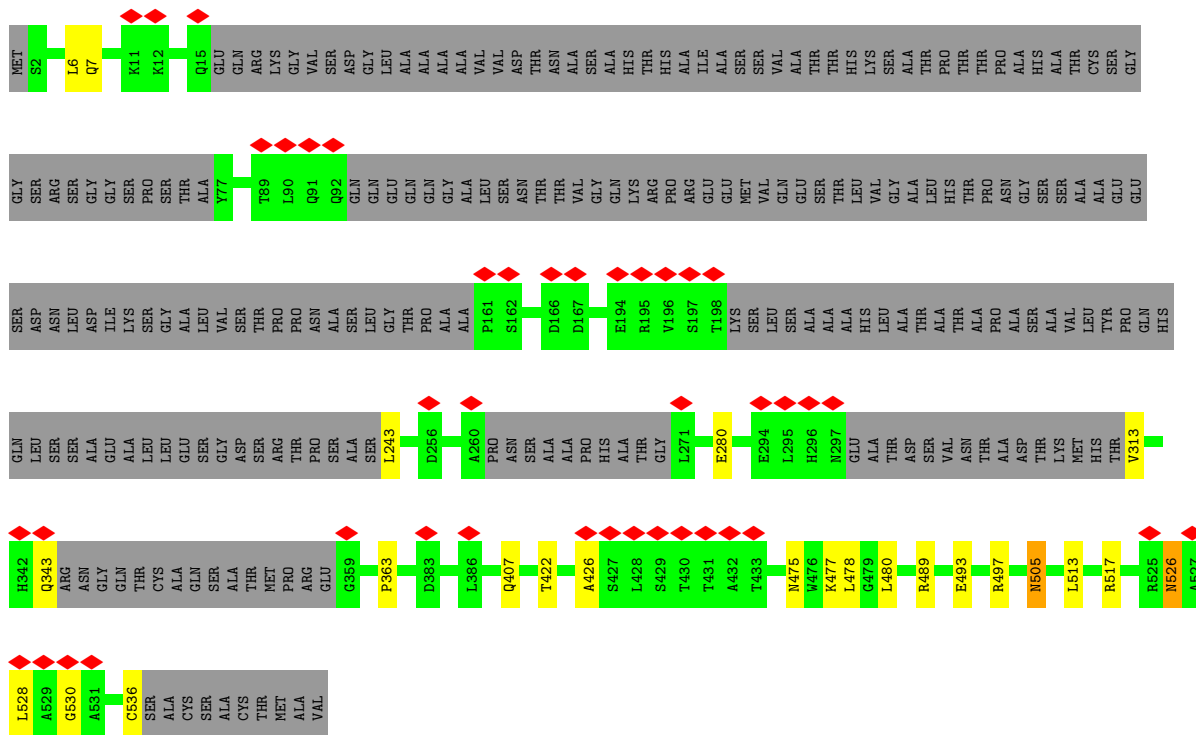
Chain SA: 86% 5% 9%



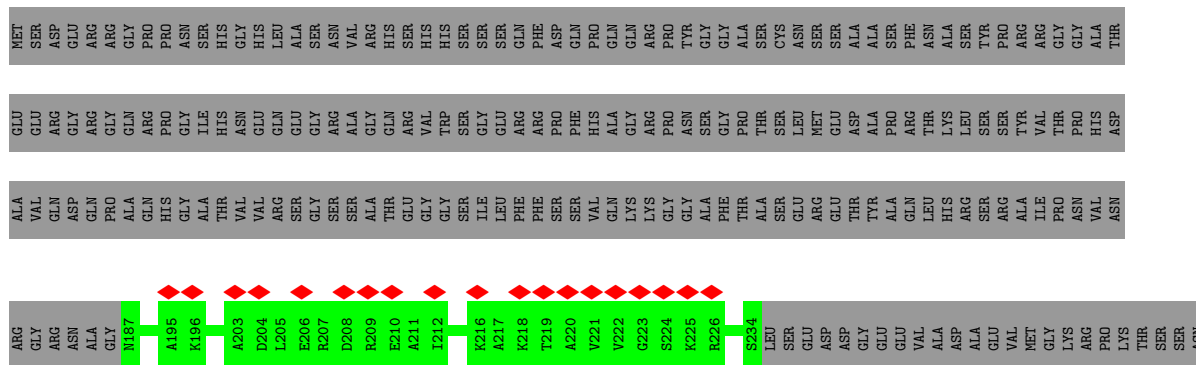
Chain SC:



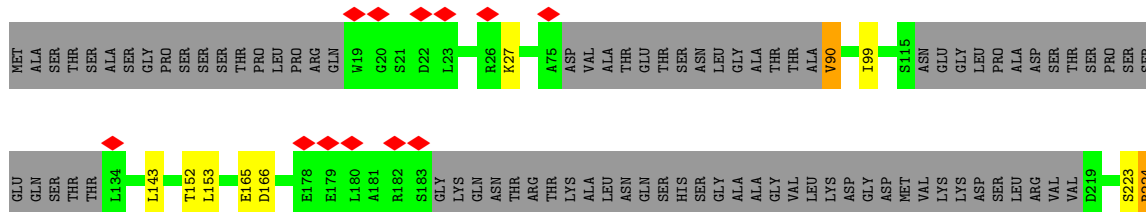
Chain SD:

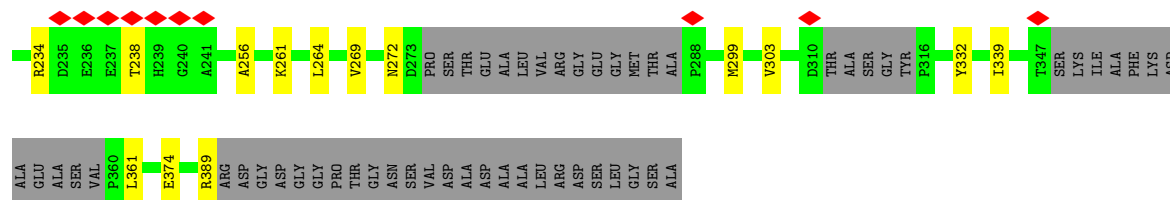


- Molecule 26: Uncharacterized protein

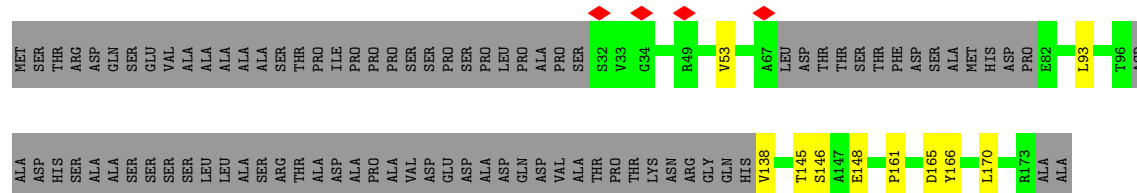


- Molecule 27: PRP19-related complex protein 3

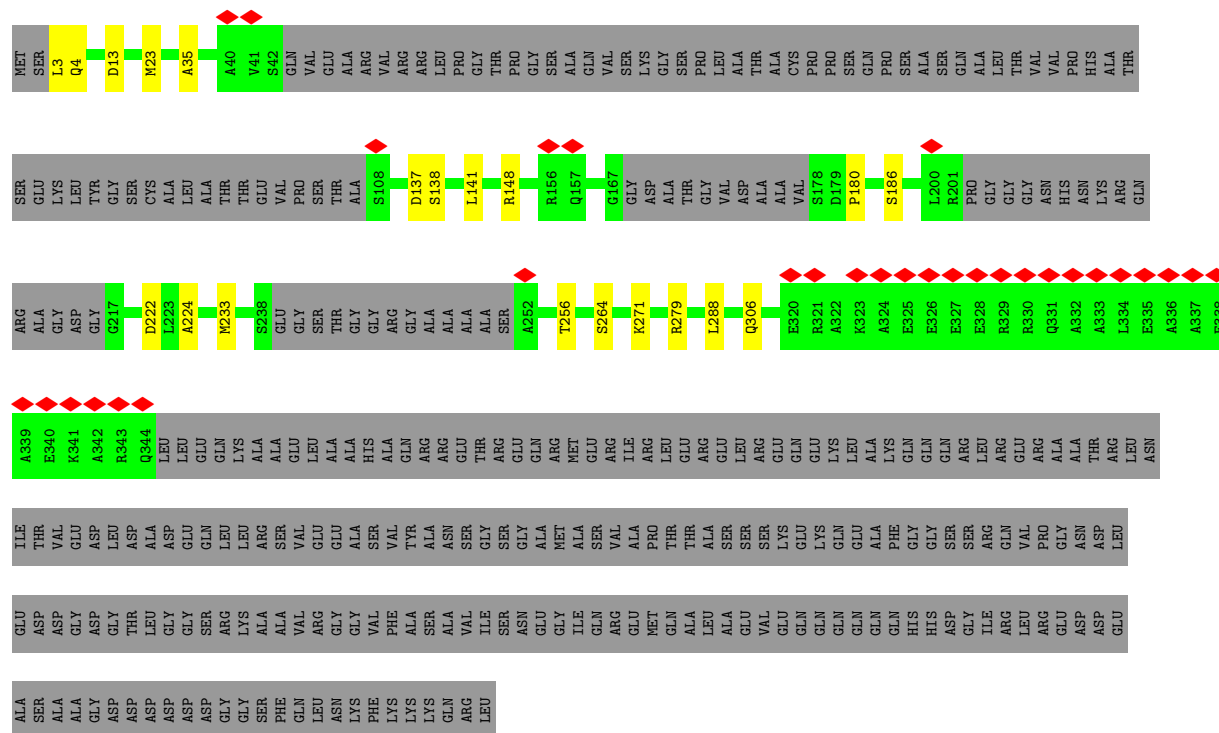
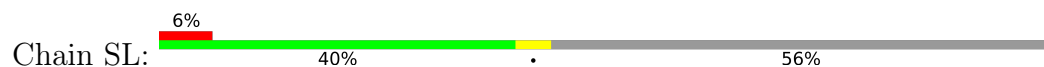




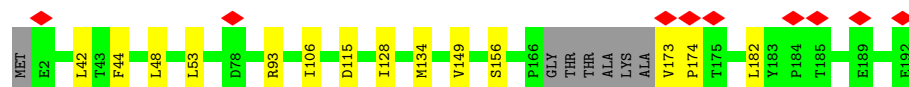
• Molecule 28: Unspecified product



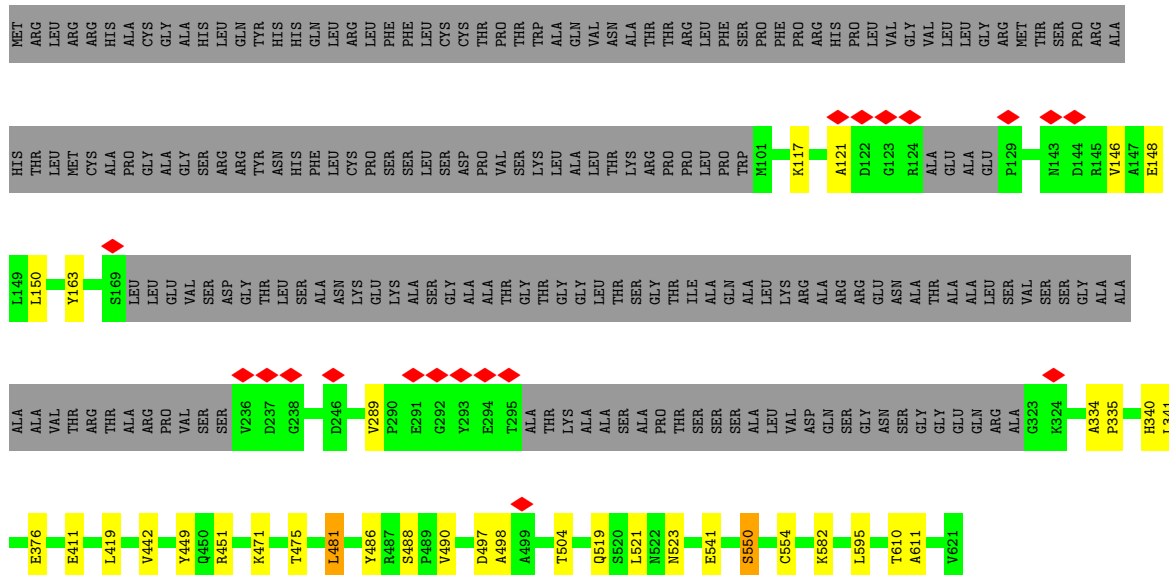
• Molecule 29: SNW domain-containing protein 1



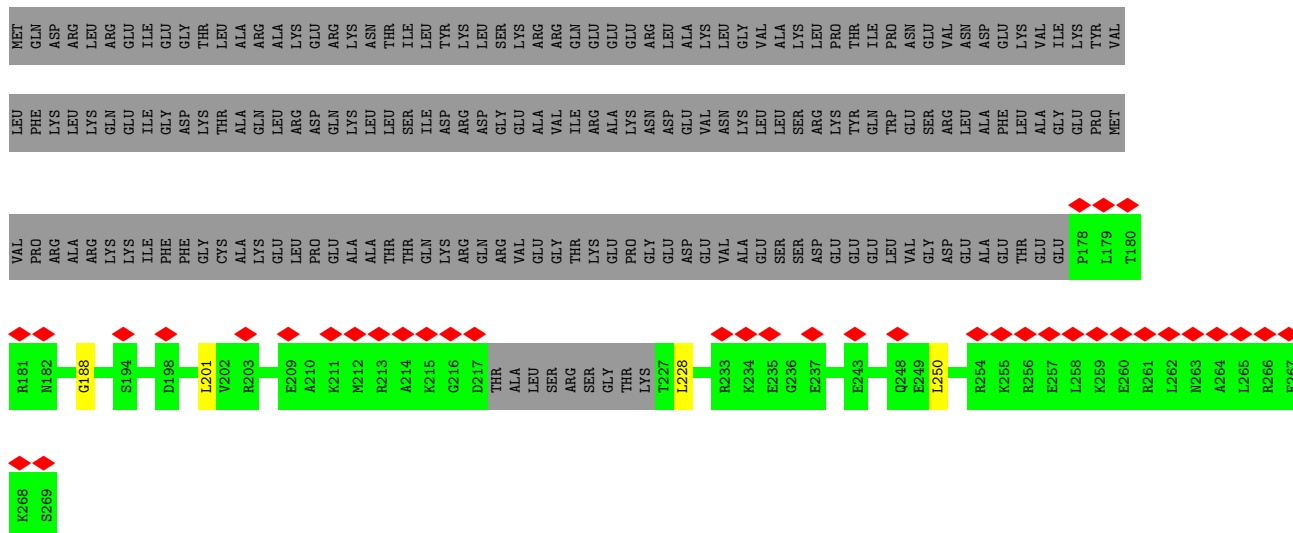
• Molecule 30: peptidylprolyl isomerase



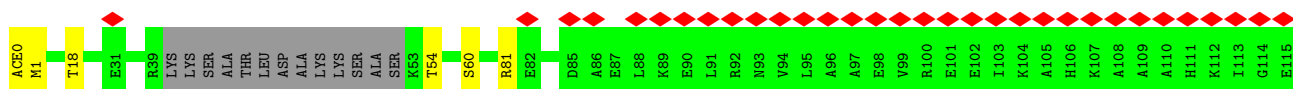
Chain SO:

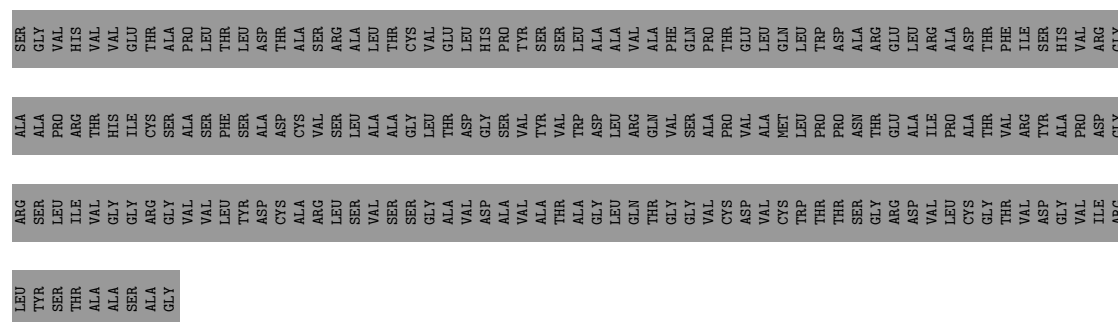


Chain SP:

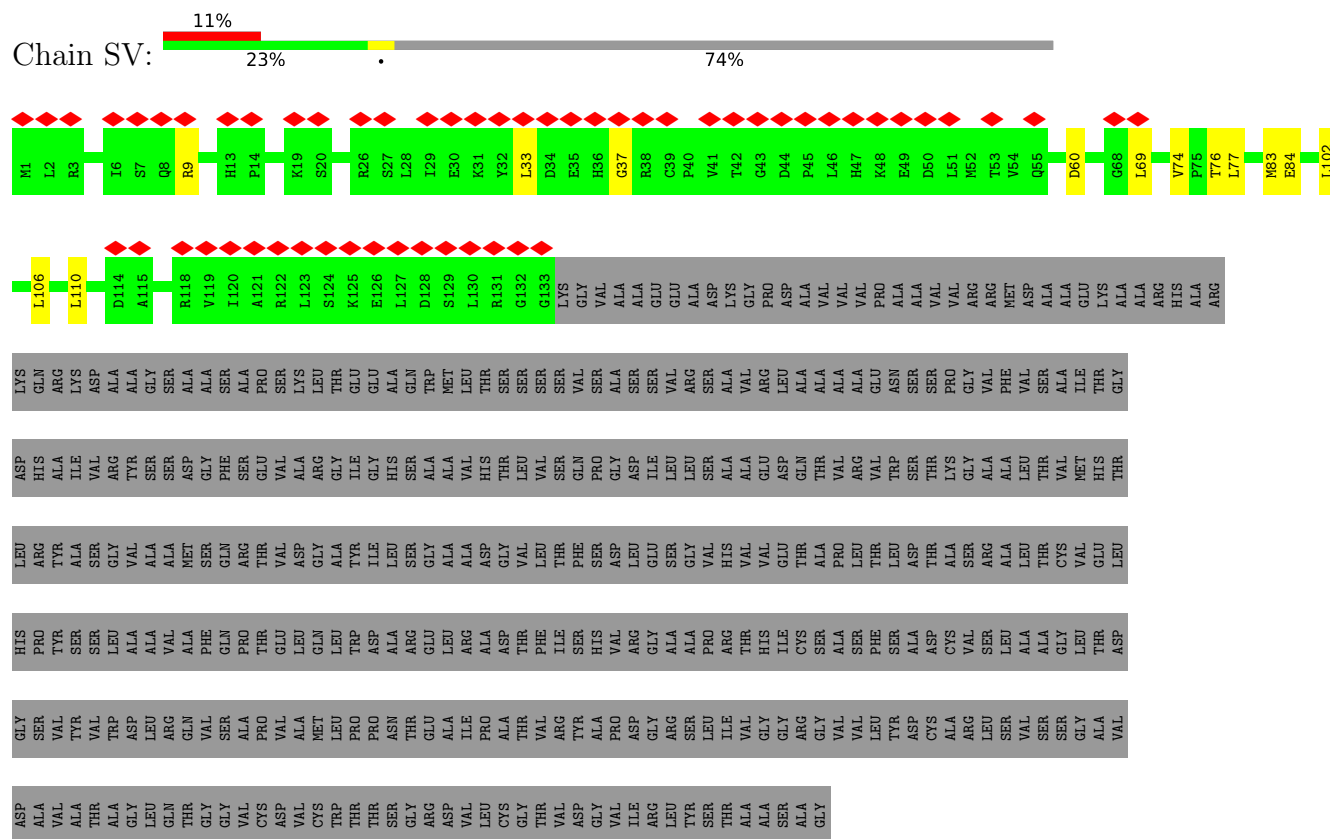


Chain SQ:

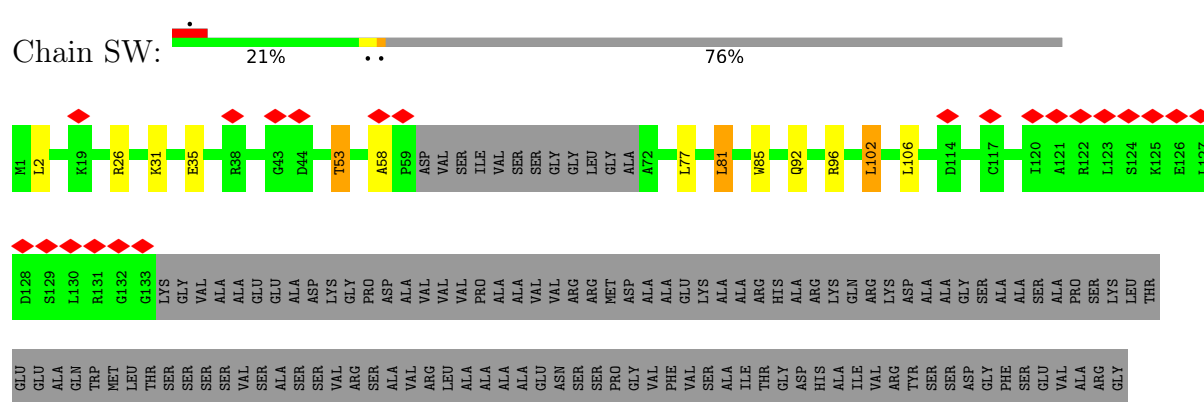




- Molecule 35: Pre-mRNA-processing factor 19



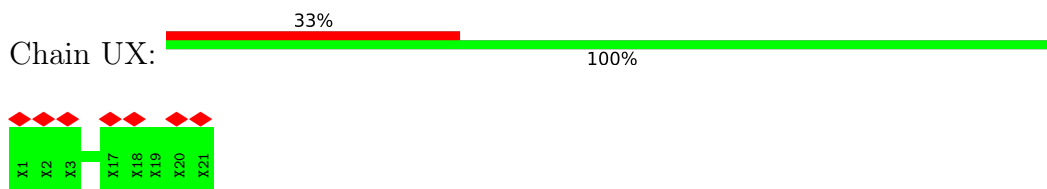
- Molecule 35: Pre-mRNA-processing factor 19



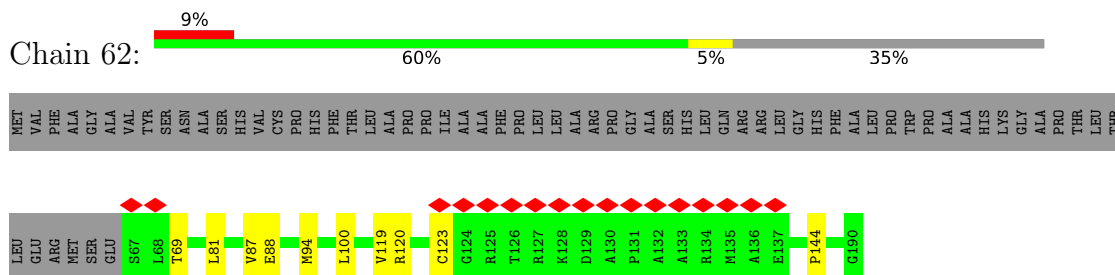


[illegible]

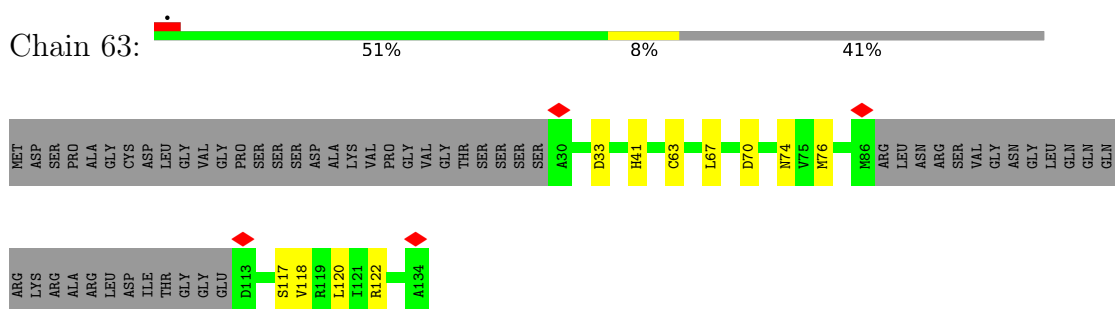
- Molecule 37: Unidentified protein



- Molecule 38: LSM domain-containing protein



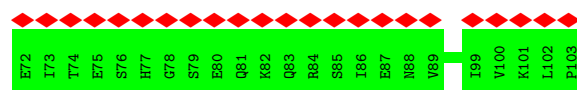
- Molecule 39: Sm domain-containing protein



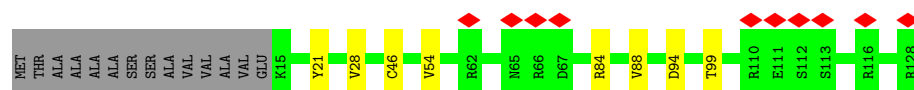
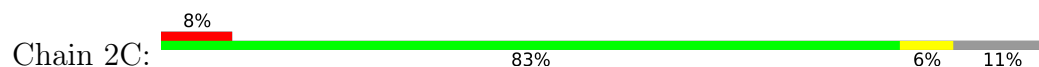
- Molecule 40: U6 snRNA-associated Sm-like protein LSm4



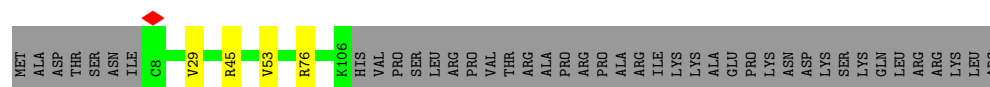
- | |
|-----|
| MET | ASP | SER | GLU | GLN | PRO | LYS | LYS | VAL | PRO | ARG | THR | GLU | THR | LYS | LYS | LEU | LEU | R21 | R22 | T23 | V24 | A25 | D26 | G27 | P28 | F29 | N30 | L31 | L32 | D33 | T34 | A35 | M36 | K37 | E38 | K39 | K40 | R41 | V42 | F43 | L52 | L53 | A54 | H55 | V56 | I57 | A58 | F59 | L65 | V66 | L67 | K68 | G69 | V70 | V71 |
|-----|



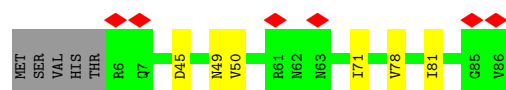
- Molecule 48: Lsm5p, putative



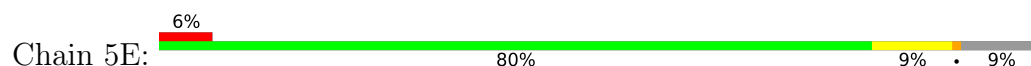
- Molecule 49: Small nuclear ribonucleoprotein, putative



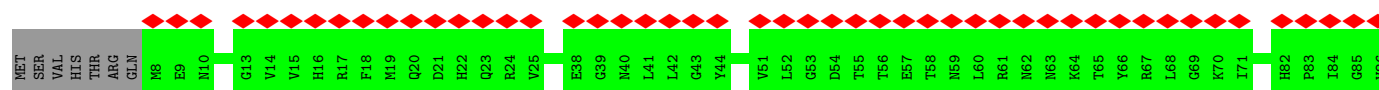
- Molecule 50: Small nuclear ribonucleoprotein E



- Molecule 50: Small nuclear ribonucleoprotein E



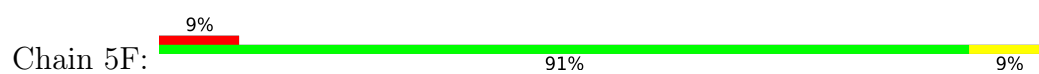
- Molecule 50: Small nuclear ribonucleoprotein E



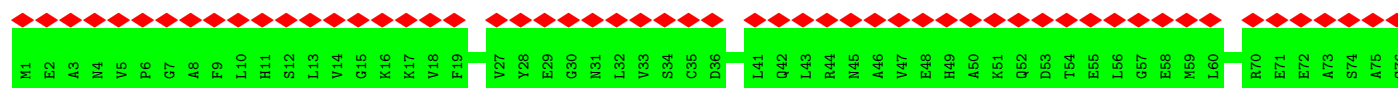
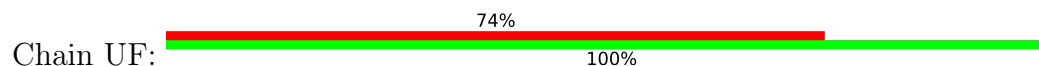
- Molecule 51: Sm protein F



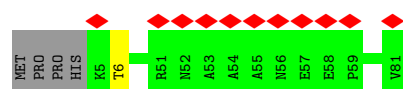
- Molecule 51: Sm protein F



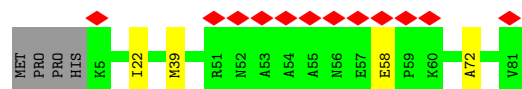
- Molecule 51: Sm protein F



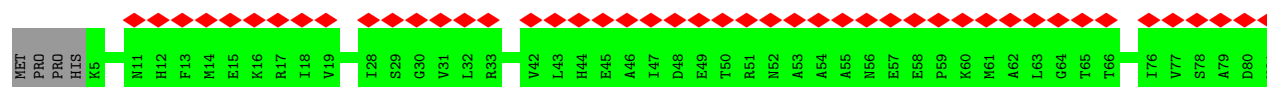
- Molecule 52: Sm protein G



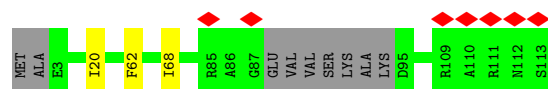
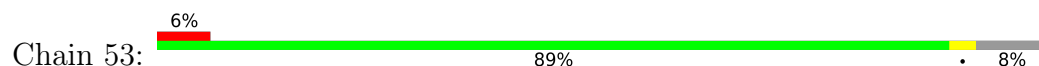
- Molecule 52: Sm protein G



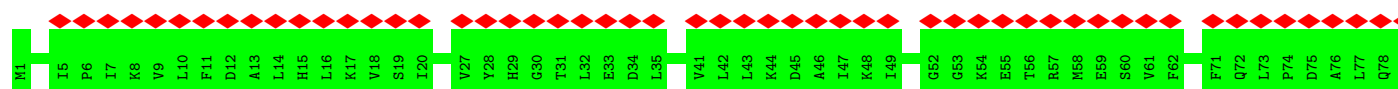
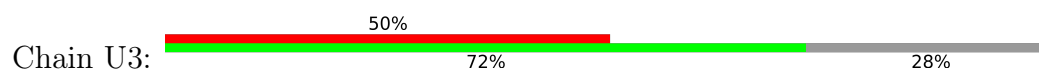
- Molecule 52: Sm protein G

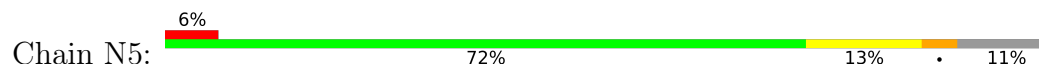


- Molecule 53: Small nuclear ribonucleoprotein Sm D3



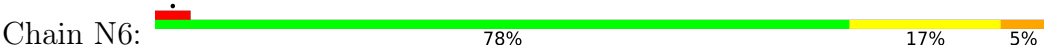
- Molecule 53: Small nuclear ribonucleoprotein Sm D3







• Molecule 59: U6 snRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	325589	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	9.611	Depositor
Minimum map value	0.000	Depositor
Average map value	0.120	Depositor
Map value standard deviation	0.210	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	426.00003, 426.00003, 426.00003	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.065, 1.065, 1.065	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: G5J, ACE, SEP, GTG, K, ZN, MG, IHP, GTP, ADP, PSU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	L7	0.18	0/3070	0.37	0/4139
2	L8	0.16	0/1023	0.34	0/1392
3	L9	0.18	0/1271	0.35	0/1715
4	LA	0.20	0/18638	0.37	0/25264
5	LB	0.13	0/10532	0.31	0/14676
6	LC	0.18	0/7137	0.35	0/9693
7	LD	0.15	0/1015	0.30	0/1351
8	LF	0.15	0/3385	0.30	0/4582
9	LG	0.11	0/600	0.24	0/810
10	LH	0.10	0/333	0.22	0/435
11	LJ	0.20	0/3268	0.36	0/4432
12	LL	0.17	0/1488	0.32	0/2008
13	LN	0.17	0/2358	0.32	0/3205
14	LP	0.20	0/617	0.36	0/826
15	LQ	0.15	0/4328	0.30	0/5818
16	LR	0.14	0/1241	0.26	0/1663
17	LS	0.16	0/6335	0.30	0/8567
18	LT	0.15	0/6427	0.29	0/8731
19	LV	0.15	0/7721	0.32	0/10452
20	LW	0.15	0/1569	0.32	0/2119
21	LY	0.17	0/895	0.29	0/1201
22	LZ	0.13	0/625	0.28	0/843
23	SA	0.16	0/4310	0.29	0/5802
24	SC	0.17	0/2147	0.31	0/2887
25	SD	0.13	0/2621	0.27	0/3538
26	SF	0.11	0/236	0.23	0/327
27	SJ	0.14	0/2240	0.29	0/3029
28	SK	0.17	0/721	0.33	0/982
29	SL	0.16	0/1774	0.30	0/2392
30	SN	0.18	0/1424	0.33	0/1940
31	SO	0.21	0/3423	0.37	0/4651
32	SP	0.12	0/690	0.26	0/918

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	SQ	0.27	1/853 (0.1%)	0.35	0/1144
34	SS	0.12	0/1526	0.27	0/2057
35	ST	0.14	0/3666	0.30	0/4992
35	SU	0.15	0/1037	0.33	0/1403
35	SV	0.15	0/1037	0.30	0/1403
35	SW	0.15	0/963	0.30	0/1301
36	TN	0.17	0/359	0.34	0/486
38	62	0.15	0/947	0.31	0/1282
39	63	0.16	0/611	0.30	0/831
40	64	0.17	0/646	0.33	0/869
41	65	0.17	0/888	0.33	0/1198
42	66	0.16	0/551	0.34	0/745
43	67	0.19	0/712	0.36	0/962
44	68	0.29	1/781 (0.1%)	0.36	0/1063
45	RN	0.17	0/74	0.34	0/111
46	24	0.14	0/792	0.27	0/1066
46	51	0.18	0/767	0.33	0/1035
46	U1	0.13	0/483	0.28	0/671
47	25	0.16	0/664	0.32	0/890
47	52	0.18	0/725	0.33	0/970
47	U2	0.10	0/410	0.29	0/570
48	2C	0.15	0/887	0.30	0/1192
49	2D	0.14	0/806	0.30	0/1086
50	2H	0.13	0/669	0.31	0/905
50	5E	0.15	0/641	0.36	0/869
50	UE	0.11	0/387	0.30	0/536
51	2I	0.16	0/608	0.34	0/818
51	5F	0.18	0/608	0.38	0/818
51	UF	0.16	0/374	0.33	0/519
52	2J	0.15	0/588	0.31	0/791
52	5G	0.14	0/588	0.29	0/791
52	UG	0.11	0/378	0.30	0/524
53	53	0.18	0/810	0.34	0/1085
53	U3	0.14	0/399	0.32	0/554
54	5B	0.18	0/745	0.37	0/997
54	UB	0.13	0/397	0.26	0/550
55	LE	0.21	0/586	0.29	0/907
56	LO	0.15	0/1124	0.25	0/1748
57	N2	0.22	0/1787	0.34	0/2774
58	N5	0.23	0/1480	0.29	0/2298
59	N6	0.22	0/2378	0.30	0/3702
All	All	0.17	2/138194 (0.0%)	0.32	0/188901

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	68	0	ACE	C-N	6.39	1.46	1.33
33	SQ	0	ACE	C-N	6.21	1.45	1.33

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L7	3021	0	3080	22	0
2	L8	999	0	956	5	0
3	L9	1243	0	1230	5	0
4	LA	18216	0	17438	88	0
5	LB	10536	0	4965	6	0
6	LC	7002	0	6999	26	0
7	LD	1006	0	1048	4	0
8	LF	3311	0	3287	23	0
9	LG	592	0	578	3	0
10	LH	331	0	354	1	0
11	LJ	3196	0	3166	31	0
12	LL	1455	0	1471	3	0
13	LN	2314	0	2243	9	0
14	LP	598	0	587	6	0
15	LQ	4277	0	4111	15	0
16	LR	1230	0	1184	8	0
17	LS	6209	0	6075	30	0
18	LT	6284	0	6228	35	0
19	LV	7589	0	7426	33	0
20	LW	1545	0	1586	3	0
21	LY	876	0	888	3	0
22	LZ	619	0	531	2	0
23	SA	4239	0	4212	14	0
24	SC	2108	0	2017	13	0
25	SD	2577	0	2581	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	SF	237	0	122	0	0
27	SJ	2197	0	2133	12	0
28	SK	699	0	675	10	0
29	SL	1770	0	1756	13	0
30	SN	1396	0	1400	11	0
31	SO	3334	0	3286	20	0
32	SP	683	0	691	1	0
33	SQ	838	0	832	3	0
34	SS	1504	0	1485	8	0
35	ST	3606	0	3602	15	0
35	SU	1022	0	1039	10	0
35	SV	1022	0	1039	7	0
35	SW	949	0	965	12	0
36	TN	351	0	361	2	0
37	UX	105	0	23	0	0
38	62	937	0	973	3	0
39	63	602	0	598	5	0
40	64	640	0	656	5	0
41	65	876	0	864	5	0
42	66	541	0	522	2	0
43	67	701	0	730	7	0
44	68	774	0	795	7	0
45	RN	283	0	178	2	0
46	24	783	0	803	4	0
46	51	758	0	777	5	0
46	U1	484	0	219	0	0
47	25	654	0	678	4	0
47	52	715	0	752	11	0
47	U2	411	0	182	0	0
48	2C	881	0	911	6	0
49	2D	792	0	807	2	0
50	2H	657	0	651	4	0
50	5E	629	0	621	11	0
50	UE	388	0	161	0	0
51	2I	598	0	597	4	0
51	5F	598	0	597	7	0
51	UF	375	0	175	0	0
52	2J	583	0	603	1	0
52	5G	583	0	603	3	0
52	UG	379	0	178	0	0
53	53	801	0	822	3	0
53	U3	400	0	181	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	5B	738	0	765	3	0
54	UB	398	0	176	0	0
55	LE	547	0	276	6	0
56	LO	1006	0	509	4	0
57	N2	1604	0	813	10	0
58	N5	1328	0	680	7	0
59	N6	2127	0	1078	14	0
60	L7	1	0	0	0	0
60	LA	1	0	0	0	0
60	LC	1	0	0	0	0
60	N5	1	0	0	0	0
60	N6	8	0	0	0	0
61	L7	27	0	12	0	0
62	L7	1	0	0	0	0
63	LA	36	0	6	2	0
64	LC	32	0	12	0	0
65	LL	3	0	0	0	0
65	SC	1	0	0	0	0
65	SQ	1	0	0	0	0
66	N5	52	0	25	0	0
67	N6	33	0	0	3	0
All	All	135855	0	123636	472	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (472) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:52:17:LYS:HE3	50:5E:47:PHE:HZ	1.11	1.09
47:52:17:LYS:HE3	50:5E:47:PHE:CZ	1.90	1.05
4:LA:415:LEU:HD22	6:LC:357:ALA:HB1	1.51	0.89
47:52:17:LYS:CE	50:5E:47:PHE:HZ	1.85	0.88
31:SO:335:PRO:HD3	31:SO:340:HIS:CE1	2.16	0.80
31:SO:475:THR:HG22	31:SO:481:LEU:HD12	1.63	0.80
48:2C:94:ASP:O	48:2C:99:THR:HG21	1.81	0.79
17:LS:352:LEU:HD23	28:SK:170:LEU:HD21	1.65	0.77
1:L7:368:ARG:NH1	3:L9:99:ASN:O	2.19	0.75
27:SJ:166:ASP:OD1	27:SJ:224:ARG:NH2	2.20	0.74
8:LF:632:THR:O	17:LS:28:ARG:NH1	2.20	0.74
4:LA:1370:ARG:NH1	58:N5:17:U:OP2	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:LF:427:GLU:OE1	8:LF:431:ARG:NH1	2.22	0.72
4:LA:1426:TYR:OH	16:LR:6:GLU:O	2.06	0.72
46:24:46:MET:SD	47:25:92:ARG:NH1	2.62	0.72
4:LA:666:ARG:NH1	63:LA:2501:IHP:O44	2.22	0.72
35:SU:3:ARG:NH2	35:SV:69:LEU:O	2.23	0.71
35:ST:248:ILE:O	35:SU:97:GLN:NE2	2.23	0.71
18:LT:310:ASP:OD1	27:SJ:27:LYS:NZ	2.19	0.70
7:LD:125:ARG:NH1	57:N2:134:G:OP1	2.24	0.70
30:SN:53:LEU:HD12	30:SN:53:LEU:O	1.92	0.70
4:LA:1565:LYS:NZ	24:SC:82:ASP:OD2	2.25	0.70
15:LQ:24:ALA:O	29:SL:279:ARG:NH1	2.25	0.70
18:LT:477:ARG:NH1	18:LT:528:ASP:OD2	2.24	0.69
17:LS:337:TYR:OH	18:LT:612:ARG:NH1	2.25	0.69
35:ST:91:GLU:OE2	35:SU:96:ARG:NH2	2.26	0.69
56:LO:41:U:O4	59:N6:42:G:O2'	2.11	0.69
11:LJ:259:ARG:NH1	11:LJ:261:GLU:OE2	2.27	0.68
18:LT:321:ASP:O	18:LT:325:LEU:N	2.26	0.68
11:LJ:170:TYR:OH	11:LJ:446:ASP:OD2	2.09	0.68
30:SN:93:ARG:NH2	31:SO:148:GLU:OE2	2.27	0.67
47:52:97:ILE:O	51:5F:65:ASN:ND2	2.27	0.67
34:SS:37:GLU:OE1	35:SU:122:ARG:NH2	2.28	0.66
39:63:122:ARG:NH2	59:N6:100:U:O2'	2.28	0.66
18:LT:543:VAL:O	27:SJ:272:ASN:ND2	2.29	0.66
6:LC:821:GLU:OE2	16:LR:69:HIS:ND1	2.28	0.66
48:2C:99:THR:HG23	48:2C:99:THR:O	1.93	0.66
4:LA:1808:MET:O	4:LA:1818:ARG:NH2	2.29	0.65
15:LQ:676:GLU:OE1	34:SS:191:ARG:NH1	2.28	0.65
4:LA:473:ASP:OD2	6:LC:957:HIS:NE2	2.30	0.65
17:LS:352:LEU:HD12	18:LT:649:LEU:HD21	1.78	0.65
19:LV:708:ILE:O	19:LV:752:ARG:NH1	2.29	0.65
11:LJ:64:ARG:NH2	35:SW:35:GLU:OE1	2.30	0.65
4:LA:717:ASP:OD1	29:SL:148:ARG:NH1	2.30	0.65
18:LT:637:HIS:O	18:LT:641:ALA:N	2.29	0.64
17:LS:743:ARG:NH2	17:LS:795:GLU:OE1	2.30	0.64
27:SJ:339:ILE:HD11	27:SJ:374:GLU:HG3	1.79	0.64
40:64:38:ARG:NH2	43:67:13:GLU:O	2.31	0.64
35:ST:2:LEU:HD23	35:SW:2:LEU:HD22	1.79	0.64
4:LA:1289:ARG:NH2	23:SA:493:GLU:O	2.30	0.63
6:LC:110:LEU:HD22	6:LC:199:HIS:CE1	2.33	0.63
6:LC:75:GLY:O	11:LJ:220:LEU:HD22	1.99	0.63
23:SA:167:ASP:OD2	23:SA:212:ARG:NH2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:ST:3:ARG:NH2	35:SW:58:ALA:O	2.31	0.63
18:LT:683:GLU:OE2	28:SK:145:THR:HG22	1.98	0.62
12:LL:212:PRO:HG3	67:N6:201:G5J:O2G	2.00	0.62
8:LF:57:ALA:O	8:LF:61:VAL:HG23	2.00	0.62
30:SN:44:PHE:CD1	30:SN:53:LEU:HD13	2.34	0.62
15:LQ:329:ARG:NH2	29:SL:288:LEU:O	2.33	0.62
34:SS:198:GLU:OE2	35:SV:9:ARG:NH1	2.33	0.62
50:2H:45:ASP:OD1	50:2H:49:ASN:N	2.33	0.62
4:LA:1439:ASN:CG	23:SA:370:ILE:HD11	2.25	0.61
35:ST:200:VAL:HG21	35:SU:83:MET:HG2	1.82	0.61
4:LA:1309:ILE:HD11	4:LA:1353:THR:HG21	1.82	0.61
15:LQ:212:GLU:OE2	31:SO:521:LEU:HD21	2.00	0.61
47:52:54:ALA:HB2	47:52:70:VAL:HA	1.82	0.61
8:LF:58:ALA:O	8:LF:62:VAL:HG23	2.00	0.61
30:SN:48:LEU:HD21	31:SO:146:VAL:HG13	1.81	0.61
17:LS:86:ARG:NH1	59:N6:75:U:O2'	2.34	0.61
19:LV:302:GLU:O	19:LV:306:GLN:N	2.33	0.61
11:LJ:302:ARG:NH1	14:LP:11:GLU:O	2.34	0.61
4:LA:1506:THR:O	4:LA:1511:ARG:NH2	2.34	0.60
59:N6:3:A:H61	59:N6:17:A:H61	1.47	0.60
4:LA:46:ASN:ND2	13:LN:120:ASN:OD1	2.34	0.60
19:LV:902:GLU:HB2	19:LV:906:LEU:HD12	1.83	0.60
5:LB:606:GLU:O	5:LB:610:ALA:N	2.33	0.60
19:LV:24:MET:HE1	19:LV:141:VAL:HG13	1.84	0.60
19:LV:191:ARG:NH1	19:LV:902:GLU:OE1	2.34	0.60
59:N6:9:U:O2'	59:N6:10:U:O5'	2.16	0.60
4:LA:1634:VAL:HG11	4:LA:1647:LEU:HD13	1.84	0.60
8:LF:124:GLU:OE1	8:LF:453:ARG:NH1	2.34	0.60
6:LC:820:GLU:OE2	16:LR:104:TYR:OH	2.20	0.60
35:ST:77:LEU:HD11	35:SW:77:LEU:O	2.01	0.60
11:LJ:157:VAL:HG22	11:LJ:455:VAL:HG11	1.83	0.59
44:68:92:ARG:NH1	59:N6:99:U:O4'	2.36	0.59
19:LV:1021:ARG:NH2	45:RN:64:N:O4'	2.34	0.59
13:LN:257:GLY:N	13:LN:262:THR:O	2.36	0.59
11:LJ:63:TRP:NE1	11:LJ:70:THR:O	2.35	0.59
17:LS:430:GLU:HG3	28:SK:170:LEU:HD12	1.83	0.59
11:LJ:283:ASP:OD2	14:LP:21:ARG:NH2	2.34	0.59
19:LV:658:LEU:O	19:LV:662:VAL:HG12	2.03	0.59
30:SN:134:MET:HE2	30:SN:149:VAL:HG11	1.84	0.59
1:L7:10:GLN:O	1:L7:46:ARG:NE	2.35	0.59
6:LC:756:PHE:CZ	6:LC:760:ILE:HD11	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:LJ:256:ASP:O	11:LJ:260:ASN:N	2.36	0.58
21:LY:46:ASN:O	57:N2:120:U:O2'	2.13	0.58
4:LA:1532:HIS:O	19:LV:210:ARG:NH2	2.37	0.58
18:LT:542:LEU:HD23	18:LT:572:MET:CE	2.33	0.58
4:LA:955:ARG:NH1	15:LQ:106:GLU:OE1	2.36	0.58
4:LA:657:ARG:NH1	58:N5:23:U:OP2	2.37	0.58
27:SJ:256:ALA:O	27:SJ:261:LYS:NZ	2.36	0.58
31:SO:595:LEU:HD11	31:SO:610:THR:HB	1.84	0.58
9:LG:60:ALA:O	9:LG:64:ASN:ND2	2.37	0.58
18:LT:716:GLN:NE2	18:LT:752:HIS:O	2.37	0.57
12:LL:87:GLU:OE2	12:LL:165:ARG:NH1	2.37	0.57
6:LC:92:LEU:HD13	11:LJ:258:GLU:OE2	2.04	0.57
35:ST:77:LEU:HD12	35:SW:81:LEU:HG	1.86	0.57
18:LT:655:ARG:NH1	29:SL:224:ALA:O	2.37	0.57
13:LN:113:ARG:NH2	67:N6:201:G5J:O1G	2.38	0.57
51:2I:52:GLN:OE1	51:2I:52:GLN:N	2.37	0.57
12:LL:215:GLU:HG2	67:N6:201:G5J:C5'	2.35	0.57
51:2I:37:THR:O	57:N2:90:A:N6	2.38	0.57
4:LA:748:LYS:NZ	57:N2:20:G:O2'	2.38	0.57
15:LQ:751:GLN:NE2	35:SV:60:ASP:OD1	2.36	0.57
50:5E:71:ILE:HG22	51:5F:70:ARG:CB	2.35	0.57
11:LJ:63:TRP:NE1	34:SS:193:CYS:SG	2.78	0.56
18:LT:136:LEU:HD12	18:LT:144:LEU:HD11	1.87	0.56
46:24:67:GLU:OE1	48:2C:21:TYR:OH	2.21	0.56
44:68:33:ILE:HD11	44:68:91:LEU:HD12	1.87	0.56
31:SO:451:ARG:NH1	31:SO:486:TYR:O	2.38	0.56
8:LF:94:LEU:O	8:LF:98:VAL:HG23	2.04	0.56
46:24:43:ASP:OD2	46:24:47:ASN:N	2.38	0.56
4:LA:164:LEU:HD23	24:SC:92:VAL:HG23	1.87	0.56
18:LT:494:LYS:NZ	41:65:69:ASP:OD2	2.38	0.56
31:SO:519:GLN:NE2	31:SO:554:CYS:O	2.38	0.56
15:LQ:399:LEU:HD13	17:LS:583:ALA:HB1	1.87	0.56
1:L7:125:THR:HG23	1:L7:149:MET:HE1	1.88	0.56
4:LA:91:LYS:NZ	56:LO:54:C:OP1	2.29	0.55
23:SA:64:LEU:O	23:SA:68:ARG:N	2.39	0.55
4:LA:1892:LEU:HD22	4:LA:1995:ILE:HG21	1.88	0.55
8:LF:389:LEU:HD23	8:LF:435:LEU:HD23	1.88	0.55
51:5F:62:ARG:NH2	58:N5:56:G:OP2	2.39	0.55
56:LO:42:A:O2'	59:N6:71:C:OP2	2.16	0.55
4:LA:905:GLN:HB2	4:LA:1501:LEU:HD21	1.89	0.55
18:LT:739:LEU:O	18:LT:756:TYR:OH	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:SO:335:PRO:HD3	31:SO:340:HIS:HE1	1.72	0.55
46:51:28:GLU:OE1	46:51:77:TYR:OH	2.20	0.55
4:LA:906:LEU:HG	4:LA:1501:LEU:HD22	1.89	0.55
11:LJ:484:ILE:HG23	11:LJ:493:LEU:HD11	1.87	0.55
23:SA:157:MET:HE2	25:SD:7:GLN:OE1	2.07	0.55
27:SJ:389:ARG:NH2	57:N2:12:G:N7	2.54	0.55
6:LC:447:LEU:HD23	6:LC:448:PRO:HD2	1.88	0.55
1:L7:20:GLU:OE2	1:L7:33:TYR:OH	2.24	0.54
4:LA:2100:ILE:HG12	22:LZ:356:MET:HE1	1.89	0.54
4:LA:736:ARG:NH2	58:N5:19:U:OP1	2.41	0.54
17:LS:422:GLN:NE2	28:SK:161:PRO:O	2.36	0.54
11:LJ:192:THR:HG22	11:LJ:203:THR:HG22	1.89	0.54
19:LV:843:GLN:OE1	19:LV:952:ARG:NH2	2.40	0.54
46:24:29:LEU:O	46:24:76:ARG:NH2	2.40	0.54
6:LC:918:ARG:NH1	6:LC:946:PHE:O	2.41	0.54
29:SL:35:ALA:HB1	31:SO:150:LEU:HD13	1.89	0.53
27:SJ:165:GLU:OE1	27:SJ:224:ARG:NH2	2.41	0.53
48:2C:94:ASP:O	48:2C:99:THR:CG2	2.56	0.53
38:62:119:VAL:HG23	38:62:144:PRO:HG3	1.91	0.53
49:2D:29:VAL:O	49:2D:76:ARG:NH2	2.42	0.53
4:LA:241:LEU:HD11	4:LA:438:ALA:HA	1.91	0.53
4:LA:1811:ASN:O	4:LA:1815:ASN:ND2	2.38	0.53
16:LR:1:MET:HE3	55:LE:29:G:H22	1.74	0.53
30:SN:174:PRO:O	35:ST:383:ARG:NH2	2.40	0.53
34:SS:186:ASN:ND2	35:SU:72:ALA:O	2.41	0.53
4:LA:439:LEU:HD22	6:LC:283:ILE:HG23	1.91	0.53
18:LT:693:ARG:NH1	29:SL:222:ASP:O	2.41	0.53
4:LA:33:GLU:OE2	4:LA:37:GLN:NE2	2.42	0.53
6:LC:498:ALA:HB2	6:LC:514:VAL:HG22	1.90	0.53
33:SQ:81:ARG:NH1	55:LE:17:G:O2'	2.42	0.53
1:L7:284:ALA:O	1:L7:297:ILE:HD13	2.09	0.53
11:LJ:421:ARG:NH1	11:LJ:439:ASP:OD1	2.42	0.53
18:LT:254:GLY:O	18:LT:258:CYS:N	2.42	0.52
30:SN:44:PHE:CD1	30:SN:53:LEU:CD1	2.92	0.52
4:LA:1751:ASN:ND2	24:SC:82:ASP:O	2.42	0.52
31:SO:117:LYS:O	31:SO:121:ALA:N	2.43	0.52
50:5E:69:GLY:O	50:5E:71:ILE:HG23	2.08	0.52
24:SC:191:VAL:HG13	24:SC:192:PHE:CD1	2.44	0.52
28:SK:146:SER:OG	28:SK:148:GLU:OE1	2.28	0.52
6:LC:71:GLU:OE1	11:LJ:180:LYS:NZ	2.42	0.52
18:LT:108:VAL:HG13	18:LT:147:VAL:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:LC:165:SER:O	6:LC:170:LYS:NZ	2.42	0.52
11:LJ:65:ALA:HB1	35:SV:83:MET:SD	2.50	0.52
4:LA:1175:ASP:OD1	4:LA:1178:ARG:NH2	2.43	0.52
17:LS:816:ARG:NH1	19:LV:120:VAL:HG13	2.25	0.52
18:LT:758:ARG:NH2	28:SK:148:GLU:OE2	2.42	0.52
50:5E:71:ILE:HG22	51:5F:70:ARG:HB3	1.92	0.52
6:LC:160:VAL:HG13	6:LC:447:LEU:HD21	1.92	0.52
34:SS:102:CYS:SG	34:SS:103:GLY:N	2.83	0.52
46:51:30:LYS:NZ	47:52:94:GLU:OE1	2.38	0.51
4:LA:220:PRO:HB2	4:LA:222:LEU:HD13	1.92	0.51
17:LS:723:GLU:O	17:LS:727:ALA:N	2.43	0.51
6:LC:5:TYR:HB3	17:LS:492:VAL:HG21	1.92	0.51
19:LV:823:ARG:O	19:LV:823:ARG:NH1	2.42	0.51
8:LF:114:ARG:NH2	8:LF:460:ASP:OD1	2.43	0.51
19:LV:844:LEU:O	19:LV:845:SER:OG	2.23	0.51
29:SL:4:GLN:OE1	44:68:104:VAL:HG22	2.11	0.51
4:LA:1111:TRP:NE1	4:LA:1115:MET:HE3	2.25	0.51
18:LT:371:ALA:HB3	27:SJ:99:ILE:HG23	1.92	0.51
27:SJ:299:MET:O	27:SJ:303:VAL:HG12	2.11	0.51
53:53:62:PHE:HE2	52:5G:39:MET:HE3	1.76	0.51
56:LO:81:G:O2'	56:LO:82:A:OP2	2.28	0.51
8:LF:655:LEU:HD22	8:LF:668:ALA:HB1	1.92	0.51
11:LJ:474:THR:HG22	14:LP:190:ASN:ND2	2.26	0.51
13:LN:173:ASP:OD1	13:LN:177:THR:N	2.44	0.51
18:LT:654:VAL:HG13	18:LT:689:THR:HG22	1.93	0.51
24:SC:296:THR:HG22	25:SD:363:PRO:HG3	1.91	0.51
46:51:71:ARG:NH2	54:5B:34:HIS:O	2.43	0.51
47:52:16:THR:OG1	50:5E:45:ASP:OD1	2.18	0.50
35:ST:119:VAL:HG12	35:SU:120:ILE:HD12	1.93	0.50
4:LA:1283:GLU:HG3	23:SA:411:MET:HE1	1.93	0.50
39:63:76:MET:HE2	39:63:118:VAL:HG12	1.92	0.50
6:LC:609:ALA:O	6:LC:613:VAL:HG23	2.12	0.50
11:LJ:474:THR:HG22	14:LP:190:ASN:HD22	1.75	0.50
4:LA:1286:TRP:HB2	4:LA:1300:ALA:HB3	1.93	0.50
23:SA:466:ARG:NE	55:LE:23:G:O6	2.44	0.50
15:LQ:774:ASP:OD2	34:SS:235:TYR:OH	2.24	0.50
17:LS:737:GLY:O	17:LS:741:ALA:N	2.45	0.50
4:LA:620:MET:HE1	4:LA:641:LEU:HB2	1.94	0.50
17:LS:609:ASP:OD1	17:LS:710:ARG:NH2	2.44	0.50
20:LW:18:MET:HE2	21:LY:24:ARG:HB2	1.94	0.50
4:LA:1870:ASP:OD1	15:LQ:198:ARG:NH2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:SU:33:LEU:O	35:SU:37:GLY:N	2.43	0.49
8:LF:634:ARG:NH1	8:LF:660:VAL:O	2.45	0.49
18:LT:500:LEU:HD21	41:65:72:ASP:C	2.38	0.49
4:LA:2111:MET:O	24:SC:258:VAL:HG11	2.13	0.49
6:LC:89:GLN:HA	6:LC:92:LEU:HD12	1.94	0.49
4:LA:1462:ARG:HB2	19:LV:213:LEU:HD13	1.94	0.49
4:LA:1915:LYS:NZ	25:SD:475:ASN:O	2.37	0.49
5:LB:1412:GLN:O	5:LB:1416:GLU:N	2.46	0.49
11:LJ:266:PHE:HZ	11:LJ:299:LEU:HD23	1.78	0.49
31:SO:541:GLU:O	31:SO:582:LYS:NZ	2.46	0.49
17:LS:426:VAL:HG11	28:SK:166:TYR:HB3	1.94	0.49
35:ST:2:LEU:HD23	35:SW:2:LEU:CD2	2.41	0.49
4:LA:723:ARG:NH2	59:N6:62:U:OP2	2.40	0.49
18:LT:495:ARG:NH1	39:63:33:ASP:OD2	2.45	0.49
29:SL:23:MET:HE1	30:SN:128:ILE:HG13	1.95	0.49
31:SO:488:SER:O	31:SO:490:VAL:N	2.46	0.49
24:SC:101:PHE:CZ	24:SC:129:VAL:HG22	2.48	0.49
1:L7:387:GLU:O	23:SA:77:ARG:NH2	2.44	0.48
1:L7:128:ASP:OD2	1:L7:145:ARG:NH1	2.45	0.48
11:LJ:484:ILE:HG12	11:LJ:495:THR:HG22	1.95	0.48
4:LA:901:LEU:HD22	4:LA:943:LEU:HD22	1.94	0.48
8:LF:52:ILE:HG23	8:LF:481:LEU:HD21	1.94	0.48
1:L7:58:ILE:HG12	1:L7:211:MET:HE1	1.95	0.48
20:LW:58:LEU:HD22	20:LW:61:PHE:HE2	1.78	0.48
31:SO:335:PRO:CD	31:SO:340:HIS:CE1	2.94	0.48
31:SO:497:ASP:OD1	31:SO:498:ALA:N	2.46	0.48
1:L7:14:LEU:HD13	1:L7:15:ALA:N	2.28	0.48
15:LQ:697:LEU:HD13	15:LQ:742:VAL:HG13	1.94	0.48
4:LA:1883:LEU:HD11	4:LA:1973:LEU:HG	1.96	0.48
11:LJ:209:ILE:HD11	11:LJ:211:LYS:HE2	1.95	0.48
19:LV:437:ASP:OD1	19:LV:465:TYR:OH	2.19	0.48
27:SJ:90:VAL:HG13	27:SJ:234:ARG:HH22	1.78	0.48
31:SO:595:LEU:HD12	31:SO:611:ALA:O	2.13	0.48
53:53:62:PHE:CE2	52:5G:39:MET:HE3	2.49	0.48
24:SC:191:VAL:HG13	24:SC:192:PHE:HD1	1.79	0.48
4:LA:1312:ILE:HG23	4:LA:1342:ILE:HD13	1.96	0.48
31:SO:523:ASN:OD1	31:SO:550:SER:OG	2.30	0.48
35:SV:33:LEU:O	35:SV:37:GLY:N	2.45	0.48
5:LB:1436:THR:O	5:LB:1496:GLY:N	2.47	0.47
40:64:69:ARG:NH2	43:67:45:ASN:OD1	2.47	0.47
30:SN:182:LEU:HD11	35:ST:378:PHE:HE2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:64:62:LYS:HB2	43:67:86:ILE:HD13	1.96	0.47
4:LA:472:PRO:HA	4:LA:475:LEU:HD22	1.97	0.47
17:LS:341:LEU:HD13	17:LS:409:ARG:NH2	2.29	0.47
47:52:54:ALA:HB3	47:52:67:LEU:HD22	1.95	0.47
4:LA:164:LEU:HD22	4:LA:682:PRO:HG3	1.96	0.47
4:LA:1362:ARG:NH2	58:N5:15:A:OP1	2.43	0.47
16:LR:1:MET:SD	16:LR:1:MET:N	2.88	0.47
4:LA:2019:ARG:NH2	8:LF:706:ARG:OXT	2.45	0.47
18:LT:599:TYR:O	18:LT:603:GLY:N	2.47	0.47
29:SL:4:GLN:CD	44:68:104:VAL:HG22	2.40	0.47
44:68:28:ASP:OD1	44:68:32:ASN:N	2.45	0.47
54:5B:44:GLU:OE1	54:5B:61:ARG:NH1	2.46	0.47
4:LA:810:GLU:OE1	11:LJ:500:LYS:NZ	2.44	0.47
18:LT:500:LEU:HD21	41:65:72:ASP:O	2.15	0.47
19:LV:24:MET:HE2	19:LV:142:GLU:HG2	1.97	0.47
4:LA:244:MET:HE3	4:LA:450:SER:O	2.15	0.47
18:LT:168:LEU:HD13	32:SP:188:GLY:HA3	1.97	0.47
19:LV:650:GLN:OE1	19:LV:653:ARG:NH2	2.48	0.47
4:LA:1482:ASP:OD1	4:LA:1483:ILE:N	2.48	0.46
18:LT:290:GLU:O	18:LT:364:ARG:NH1	2.48	0.46
19:LV:521:ASP:OD2	19:LV:552:THR:OG1	2.33	0.46
46:51:74:THR:HG21	54:5B:74:VAL:HA	1.97	0.46
50:5E:19:MET:HE3	51:5F:1:MET:HE3	1.96	0.46
8:LF:597:THR:O	8:LF:602:ASN:ND2	2.48	0.46
1:L7:316:ALA:O	1:L7:345:ARG:NE	2.49	0.46
28:SK:165:ASP:OD1	28:SK:166:TYR:N	2.49	0.46
30:SN:53:LEU:HD12	30:SN:53:LEU:C	2.41	0.46
4:LA:157:ARG:NH2	4:LA:678:VAL:O	2.48	0.46
10:LH:154:GLN:NE2	18:LT:321:ASP:OD2	2.47	0.46
19:LV:525:LEU:HG	19:LV:797:MET:HE1	1.98	0.46
40:64:65:GLU:OE2	43:67:17:SER:OG	2.33	0.46
4:LA:1965:LEU:HD13	4:LA:2091:LEU:O	2.16	0.46
35:SW:92:GLN:OE1	35:SW:96:ARG:NH1	2.49	0.46
41:65:74:LEU:CD2	42:66:3:VAL:HG21	2.46	0.46
19:LV:997:ARG:NH2	19:LV:1026:GLU:OE2	2.49	0.46
18:LT:663:VAL:HG21	29:SL:233:MET:HG2	1.96	0.46
9:LG:9:ASN:ND2	9:LG:74:PHE:O	2.48	0.46
17:LS:411:LEU:HD22	17:LS:428:VAL:HG22	1.98	0.46
1:L7:117:TYR:OH	1:L7:128:ASP:OD1	2.32	0.46
39:63:70:ASP:OD1	39:63:74:ASN:N	2.46	0.46
13:LN:1:MET:SD	13:LN:1:MET:N	2.76	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:SC:197:ALA:HB2	25:SD:497:ARG:HG2	1.98	0.45
4:LA:917:ILE:HD11	4:LA:929:GLN:HG2	1.97	0.45
19:LV:641:GLN:O	19:LV:885:ARG:NH2	2.50	0.45
47:52:17:LYS:CE	50:5E:47:PHE:CZ	2.74	0.45
1:L7:253:LEU:O	23:SA:45:ASN:ND2	2.43	0.45
4:LA:124:VAL:HG22	4:LA:544:LYS:HG2	1.99	0.45
8:LF:687:PHE:O	17:LS:27:GLY:N	2.45	0.45
25:SD:280:GLU:OE2	25:SD:407:GLN:NE2	2.48	0.45
1:L7:334:LEU:HD13	55:LE:17:G:N2	2.32	0.45
4:LA:438:ALA:HB1	6:LC:401:VAL:HG12	1.99	0.45
23:SA:62:GLU:OE2	33:SQ:60:SER:OG	2.35	0.45
35:ST:339:THR:O	35:ST:343:ALA:HB2	2.16	0.45
38:62:88:GLU:OE2	38:62:120:ARG:NE	2.48	0.45
1:L7:388:GLN:OE1	2:L8:90:CYS:SG	2.64	0.45
8:LF:685:ILE:HG12	17:LS:23:VAL:HG12	1.99	0.45
20:LW:153:ARG:NH1	20:LW:166:ILE:O	2.47	0.45
49:2D:45:ARG:NH2	52:2J:6:THR:O	2.45	0.45
1:L7:287:GLY:N	55:LE:20:U:OP1	2.45	0.45
4:LA:777:GLU:OE1	29:SL:264:SER:OG	2.22	0.45
44:68:11:SER:HB2	44:68:102:ILE:HD11	1.99	0.45
47:25:62:HIS:CE1	57:N2:89:A:H1'	2.51	0.45
1:L7:222:ASP:OD2	3:L9:62:ILE:HG21	2.16	0.45
5:LB:1449:TRP:O	5:LB:1453:PHE:N	2.49	0.45
6:LC:482:GLU:HB3	6:LC:485:ALA:HB3	1.99	0.45
4:LA:100:ILE:HD13	4:LA:563:MET:SD	2.56	0.45
7:LD:38:TYR:CE2	7:LD:42:ILE:HD11	2.52	0.45
8:LF:428:ALA:O	8:LF:432:LEU:N	2.50	0.45
18:LT:612:ARG:O	18:LT:616:SER:N	2.48	0.45
36:TN:15:MET:SD	36:TN:16:VAL:N	2.90	0.45
48:2C:99:THR:O	48:2C:99:THR:CG2	2.63	0.45
4:LA:124:VAL:HG23	4:LA:135:ASP:HB2	1.99	0.44
35:ST:409:ASP:OD2	35:ST:411:SER:OG	2.31	0.44
11:LJ:484:ILE:CG2	11:LJ:493:LEU:HD11	2.47	0.44
17:LS:617:HIS:HA	17:LS:620:THR:HG22	1.99	0.44
22:LZ:395:GLN:O	22:LZ:399:SER:N	2.49	0.44
1:L7:132:LEU:HD22	1:L7:155:LEU:HD13	1.97	0.44
4:LA:927:GLU:OE2	4:LA:931:ARG:NE	2.50	0.44
8:LF:584:MET:O	8:LF:665:ALA:N	2.49	0.44
17:LS:742:LEU:HD23	17:LS:794:PHE:CG	2.52	0.44
8:LF:435:LEU:HD21	19:LV:141:VAL:HA	2.00	0.44
23:SA:144:ASP:OD1	23:SA:251:ARG:NE	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:5E:74:ARG:NH1	51:5F:39:MET:SD	2.91	0.44
4:LA:362:ASP:O	4:LA:436:LYS:NZ	2.50	0.44
13:LN:3:LEU:HD23	13:LN:24:GLY:HA3	2.00	0.44
23:SA:301:GLN:OE1	33:SQ:54:THR:HG22	2.17	0.44
39:63:76:MET:HE3	39:63:120:LEU:HB2	1.99	0.44
19:LV:984:ASP:OD2	19:LV:985:SER:N	2.51	0.44
35:ST:14:PRO:HG3	35:SW:2:LEU:HD11	2.00	0.44
42:66:7:SER:O	42:66:11:GLN:NE2	2.51	0.44
15:LQ:764:ARG:NH2	34:SS:231:GLU:OE2	2.45	0.44
21:LY:16:LYS:NZ	57:N2:115:G:N7	2.66	0.44
30:SN:115:ASP:OD2	31:SO:163:TYR:OH	2.31	0.44
4:LA:1925:ARG:HH11	25:SD:478:LEU:HD22	1.83	0.44
4:LA:1286:TRP:CD2	4:LA:1302:LEU:HD11	2.53	0.44
31:SO:334:ALA:O	31:SO:341:LEU:HB2	2.18	0.44
8:LF:685:ILE:HG23	8:LF:695:LEU:HD13	2.00	0.43
19:LV:637:PHE:O	19:LV:719:SER:OG	2.19	0.43
50:5E:30:VAL:HG22	52:5G:72:ALA:HB2	1.99	0.43
17:LS:478:ASP:OD1	17:LS:478:ASP:N	2.48	0.43
29:SL:137:ASP:OD1	29:SL:138:SER:N	2.50	0.43
35:ST:369:ASP:O	35:ST:373:LEU:N	2.48	0.43
47:25:70:VAL:HG21	47:25:89:VAL:HB	1.99	0.43
4:LA:1671:LEU:HD21	4:LA:1796:MET:HE1	2.00	0.43
6:LC:477:ALA:HB3	6:LC:486:ALA:HB2	1.99	0.43
18:LT:196:LEU:HD12	18:LT:238:TRP:HH2	1.83	0.43
19:LV:503:THR:HG23	19:LV:508:ASP:CG	2.42	0.43
8:LF:249:LEU:CD2	8:LF:449:VAL:HG23	2.49	0.43
4:LA:1934:SER:OG	24:SC:248:ARG:NH2	2.52	0.43
11:LJ:66:LEU:HD22	35:SU:64:VAL:HB	2.00	0.43
50:2H:71:ILE:HG22	51:2I:70:ARG:HB3	2.00	0.43
4:LA:71:ILE:HD13	4:LA:125:TYR:CD1	2.54	0.43
19:LV:608:THR:HG22	36:TN:9:THR:CG2	2.49	0.43
17:LS:352:LEU:HD23	28:SK:170:LEU:CD2	2.44	0.43
18:LT:335:GLN:O	18:LT:339:GLY:N	2.52	0.43
43:67:8:VAL:HG13	43:67:12:LYS:O	2.19	0.43
47:25:62:HIS:CE1	57:N2:89:A:C1'	3.02	0.43
35:SV:102:LEU:HB3	35:SW:102:LEU:HD12	2.01	0.43
4:LA:1957:ASN:ND2	24:SC:206:GLU:OE1	2.48	0.43
11:LJ:381:LYS:O	11:LJ:385:GLY:N	2.48	0.43
6:LC:915:LEU:O	6:LC:920:GLY:N	2.47	0.43
13:LN:136:ASP:OD1	13:LN:137:GLY:N	2.52	0.43
16:LR:47:ILE:C	16:LR:47:ILE:HD12	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:LV:191:ARG:NH2	19:LV:900:GLN:OE1	2.46	0.43
24:SC:46:SER:OG	24:SC:49:ILE:HG13	2.19	0.43
17:LS:201:LEU:HD22	27:SJ:303:VAL:HG11	2.00	0.42
4:LA:190:LEU:O	4:LA:625:ARG:NH1	2.48	0.42
15:LQ:276:MET:HG2	17:LS:63:ILE:HD11	2.01	0.42
18:LT:402:ILE:HG23	18:LT:420:PHE:CZ	2.54	0.42
18:LT:682:LEU:O	18:LT:685:SER:OG	2.34	0.42
2:L8:14:LEU:HD11	2:L8:40:PRO:HG2	2.01	0.42
4:LA:241:LEU:HD12	4:LA:441:LEU:HD12	2.00	0.42
6:LC:847:LEU:O	6:LC:1003:ARG:NH1	2.46	0.42
16:LR:47:ILE:HD12	16:LR:47:ILE:O	2.19	0.42
1:L7:56:ASP:HB3	1:L7:211:MET:HE3	2.01	0.42
11:LJ:349:ARG:NH2	29:SL:180:PRO:O	2.53	0.42
2:L8:128:ALA:CB	3:L9:71:VAL:HG21	2.48	0.42
4:LA:1757:ARG:NH2	24:SC:87:GLU:OE2	2.52	0.42
19:LV:557:ALA:HB1	19:LV:804:LEU:HD22	2.01	0.42
4:LA:1918:GLU:HA	4:LA:1950:MET:HE2	2.01	0.42
8:LF:135:ILE:O	8:LF:139:VAL:HG23	2.19	0.42
25:SD:422:THR:O	25:SD:426:ALA:N	2.53	0.42
1:L7:184:TYR:OH	16:LR:125:LYS:O	2.29	0.42
4:LA:664:ARG:NH2	58:N5:5:C:OP1	2.52	0.42
4:LA:764:LYS:NZ	57:N2:16:U:OP1	2.51	0.42
25:SD:505:ASN:OD1	25:SD:505:ASN:N	2.52	0.42
4:LA:838:LEU:HD13	4:LA:965:ASP:HB2	2.00	0.42
7:LD:71:GLU:OE2	31:SO:471:LYS:NZ	2.45	0.42
15:LQ:223:LEU:HD22	15:LQ:227:GLN:HB2	2.01	0.42
17:LS:163:VAL:HG13	27:SJ:332:TYR:HB2	2.02	0.42
48:2C:28:VAL:HG13	48:2C:88:VAL:HG13	2.02	0.42
4:LA:732:LYS:NZ	59:N6:56:U:OP2	2.52	0.42
17:LS:298:VAL:HG13	17:LS:304:LEU:HB3	2.01	0.42
1:L7:265:ARG:NH1	55:LE:20:U:OP2	2.48	0.42
11:LJ:6:MET:HE1	35:SV:110:LEU:HD12	2.02	0.42
15:LQ:400:PHE:HZ	17:LS:551:ILE:HG21	1.85	0.42
4:LA:552:ALA:O	4:LA:556:VAL:HG23	2.20	0.41
6:LC:608:ALA:HB1	6:LC:626:ALA:HB2	2.02	0.41
15:LQ:23:LEU:HD22	15:LQ:28:LEU:HD23	2.02	0.41
2:L8:99:GLU:OE1	3:L9:160:LYS:NZ	2.52	0.41
4:LA:1286:TRP:CE2	4:LA:1302:LEU:HD11	2.54	0.41
19:LV:531:ASP:OD1	19:LV:533:SER:OG	2.34	0.41
58:N5:20:U:H4'	59:N6:65:G:H22	1.85	0.41
4:LA:964:MET:HB2	4:LA:973:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L8:80:THR:OG1	3:L9:160:LYS:NZ	2.53	0.41
7:LD:52:ARG:NH2	45:RN:4:N:O4'	2.52	0.41
8:LF:256:LEU:HG	8:LF:445:ALA:HB1	2.01	0.41
19:LV:670:MET:O	19:LV:697:VAL:N	2.48	0.41
9:LG:20:LEU:HD22	9:LG:29:VAL:HG11	2.03	0.41
13:LN:3:LEU:HD21	13:LN:49:LEU:HD22	2.02	0.41
14:LP:11:GLU:HG3	59:N6:66:C:N3	2.36	0.41
35:SW:26:ARG:NH2	35:SW:53:THR:OG1	2.47	0.41
50:2H:78:VAL:CG1	50:2H:81:ILE:HD11	2.51	0.41
1:L7:307:ARG:NH2	23:SA:44:VAL:O	2.54	0.41
11:LJ:340:ASP:O	11:LJ:344:GLY:N	2.50	0.41
19:LV:662:VAL:HG22	19:LV:664:THR:H	1.85	0.41
44:68:30:LEU:HD13	59:N6:99:U:C4	2.56	0.41
50:2H:78:VAL:HG11	50:2H:81:ILE:HD11	2.03	0.41
1:L7:84:ARG:NH2	6:LC:970:ASP:OD2	2.54	0.41
4:LA:644:HIS:NE2	63:LA:2501:IHP:O43	2.51	0.41
4:LA:1351:LEU:HD22	23:SA:370:ILE:CG2	2.51	0.41
5:LB:620:GLU:N	5:LB:656:LEU:O	2.54	0.41
18:LT:599:TYR:CD2	28:SK:93:LEU:HD13	2.55	0.41
19:LV:915:TRP:CG	19:LV:935:LEU:HD13	2.55	0.41
5:LB:1805:ASN:O	5:LB:1809:ALA:N	2.52	0.41
11:LJ:270:LYS:NZ	59:N6:57:C:OP2	2.50	0.41
17:LS:521:ALA:HB2	17:LS:527:PRO:HD3	2.03	0.41
19:LV:284:LEU:O	19:LV:288:ALA:HB3	2.20	0.41
4:LA:659:MET:CE	4:LA:1623:ALA:HB2	2.52	0.40
6:LC:923:LEU:N	6:LC:937:ARG:O	2.53	0.40
11:LJ:153:SER:O	11:LJ:157:VAL:HG23	2.21	0.40
19:LV:619:LEU:HD22	19:LV:651:LEU:HG	2.02	0.40
25:SD:526:ASN:O	25:SD:530:GLY:N	2.51	0.40
35:SU:78:LEU:HD11	35:SW:85:TRP:CD1	2.56	0.40
38:62:94:MET:HE2	38:62:120:ARG:HB2	2.03	0.40
46:51:84:LEU:O	47:52:88:ASN:ND2	2.55	0.40
59:N6:15:G:H3'	59:N6:16:G:H21	1.86	0.40
4:LA:318:ASN:ND2	4:LA:320:ARG:O	2.54	0.40
4:LA:877:MET:SD	14:LP:162:LEU:HD12	2.61	0.40
8:LF:34:MET:HE2	8:LF:102:SER:CB	2.50	0.40
40:64:69:ARG:NH1	43:67:72:GLY:O	2.55	0.40
51:2I:63:ASN:OD1	51:2I:64:ASN:N	2.54	0.40
47:52:98:PHE:CD1	51:5F:59:MET:HE2	2.56	0.40
53:53:20:ILE:CG2	53:53:68:ILE:HG23	2.51	0.40
4:LA:123:VAL:HG13	4:LA:132:THR:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:LA:1670:LYS:HG3	4:LA:1803:LEU:HD13	2.02	0.40
4:LA:1087:LYS:NZ	57:N2:23:A:O2'	2.54	0.40
11:LJ:61:VAL:HG13	35:SW:31:LYS:HD3	2.02	0.40
13:LN:43:ASP:OD1	13:LN:47:ALA:N	2.54	0.40
17:LS:232:TYR:O	17:LS:235:THR:OG1	2.38	0.40
18:LT:492:ALA:HB1	18:LT:495:ARG:HB3	2.04	0.40
4:LA:801:VAL:O	4:LA:805:VAL:HG23	2.22	0.40
4:LA:905:GLN:CB	4:LA:1501:LEU:HD21	2.51	0.40
41:65:33:MET:HE2	43:67:5:ALA:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L7	380/389 (98%)	375 (99%)	5 (1%)	0	100	100
2	L8	123/153 (80%)	122 (99%)	1 (1%)	0	100	100
3	L9	150/162 (93%)	149 (99%)	1 (1%)	0	100	100
4	LA	2341/2427 (96%)	2306 (98%)	35 (2%)	0	100	100
5	LB	2120/2367 (90%)	2095 (99%)	25 (1%)	0	100	100
6	LC	901/1016 (89%)	890 (99%)	11 (1%)	0	100	100
7	LD	123/166 (74%)	123 (100%)	0	0	100	100
8	LF	398/706 (56%)	396 (100%)	2 (0%)	0	100	100
9	LG	78/82 (95%)	78 (100%)	0	0	100	100
10	LH	38/159 (24%)	38 (100%)	0	0	100	100
11	LJ	405/509 (80%)	401 (99%)	4 (1%)	0	100	100
12	LL	182/326 (56%)	179 (98%)	3 (2%)	0	100	100
13	LN	312/322 (97%)	303 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	LP	69/207 (33%)	68 (99%)	1 (1%)	0	100	100
15	LQ	535/804 (66%)	532 (99%)	3 (1%)	0	100	100
16	LR	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
17	LS	768/824 (93%)	760 (99%)	8 (1%)	0	100	100
18	LT	792/794 (100%)	790 (100%)	2 (0%)	0	100	100
19	LV	967/1087 (89%)	953 (99%)	14 (1%)	0	100	100
20	LW	184/307 (60%)	182 (99%)	2 (1%)	0	100	100
21	LY	105/114 (92%)	105 (100%)	0	0	100	100
22	LZ	87/403 (22%)	86 (99%)	1 (1%)	0	100	100
23	SA	505/564 (90%)	500 (99%)	5 (1%)	0	100	100
24	SC	255/417 (61%)	251 (98%)	4 (2%)	0	100	100
25	SD	308/546 (56%)	303 (98%)	5 (2%)	0	100	100
26	SF	46/258 (18%)	46 (100%)	0	0	100	100
27	SJ	259/414 (63%)	258 (100%)	1 (0%)	0	100	100
28	SK	81/175 (46%)	80 (99%)	1 (1%)	0	100	100
29	SL	228/544 (42%)	224 (98%)	4 (2%)	0	100	100
30	SN	181/192 (94%)	178 (98%)	3 (2%)	0	100	100
31	SO	416/621 (67%)	405 (97%)	11 (3%)	0	100	100
32	SP	79/269 (29%)	79 (100%)	0	0	100	100
33	SQ	102/150 (68%)	101 (99%)	1 (1%)	0	100	100
34	SS	178/284 (63%)	176 (99%)	2 (1%)	0	100	100
35	ST	482/513 (94%)	473 (98%)	9 (2%)	0	100	100
35	SU	131/513 (26%)	129 (98%)	2 (2%)	0	100	100
35	SV	131/513 (26%)	130 (99%)	1 (1%)	0	100	100
35	SW	117/513 (23%)	115 (98%)	2 (2%)	0	100	100
36	TN	42/1181 (4%)	40 (95%)	2 (5%)	0	100	100
38	62	122/190 (64%)	122 (100%)	0	0	100	100
39	63	75/134 (56%)	75 (100%)	0	0	100	100
40	64	81/116 (70%)	81 (100%)	0	0	100	100
41	65	108/151 (72%)	105 (97%)	3 (3%)	0	100	100
42	66	69/80 (86%)	69 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	67	89/91 (98%)	86 (97%)	3 (3%)	0	100	100
44	68	98/131 (75%)	98 (100%)	0	0	100	100
46	24	100/102 (98%)	100 (100%)	0	0	100	100
46	51	96/102 (94%)	96 (100%)	0	0	100	100
46	U1	96/102 (94%)	96 (100%)	0	0	100	100
47	25	80/103 (78%)	78 (98%)	2 (2%)	0	100	100
47	52	87/103 (84%)	86 (99%)	1 (1%)	0	100	100
47	U2	81/103 (79%)	81 (100%)	0	0	100	100
48	2C	112/128 (88%)	111 (99%)	1 (1%)	0	100	100
49	2D	97/141 (69%)	97 (100%)	0	0	100	100
50	2H	79/86 (92%)	77 (98%)	2 (2%)	0	100	100
50	5E	76/86 (88%)	73 (96%)	3 (4%)	0	100	100
50	UE	77/86 (90%)	76 (99%)	1 (1%)	0	100	100
51	2I	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
51	5F	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
51	UF	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
52	2J	75/81 (93%)	75 (100%)	0	0	100	100
52	5G	75/81 (93%)	75 (100%)	0	0	100	100
52	UG	75/81 (93%)	75 (100%)	0	0	100	100
53	53	100/113 (88%)	98 (98%)	2 (2%)	0	100	100
53	U3	79/113 (70%)	78 (99%)	1 (1%)	0	100	100
54	5B	97/111 (87%)	94 (97%)	3 (3%)	0	100	100
54	UB	79/111 (71%)	77 (98%)	2 (2%)	0	100	100
All	All	17179/24142 (71%)	16968 (99%)	211 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L7	329/336 (98%)	319 (97%)	10 (3%)	36	66
2	L8	108/130 (83%)	108 (100%)	0	100	100
3	L9	139/146 (95%)	134 (96%)	5 (4%)	31	60
4	LA	1824/2116 (86%)	1771 (97%)	53 (3%)	37	67
6	LC	751/831 (90%)	719 (96%)	32 (4%)	26	54
7	LD	104/136 (76%)	102 (98%)	2 (2%)	50	77
8	LF	353/584 (60%)	330 (94%)	23 (6%)	15	37
9	LG	59/61 (97%)	58 (98%)	1 (2%)	53	79
10	LH	33/133 (25%)	32 (97%)	1 (3%)	36	66
11	LJ	336/414 (81%)	316 (94%)	20 (6%)	17	41
12	LL	154/268 (58%)	151 (98%)	3 (2%)	50	77
13	LN	240/243 (99%)	215 (90%)	25 (10%)	7	17
14	LP	63/171 (37%)	60 (95%)	3 (5%)	23	50
15	LQ	416/657 (63%)	400 (96%)	16 (4%)	29	58
16	LR	118/149 (79%)	117 (99%)	1 (1%)	73	88
17	LS	624/665 (94%)	598 (96%)	26 (4%)	26	55
18	LT	661/661 (100%)	645 (98%)	16 (2%)	43	72
19	LV	808/940 (86%)	782 (97%)	26 (3%)	34	64
20	LW	175/273 (64%)	171 (98%)	4 (2%)	44	73
21	LY	90/97 (93%)	86 (96%)	4 (4%)	25	53
22	LZ	47/321 (15%)	47 (100%)	0	100	100
23	SA	458/496 (92%)	447 (98%)	11 (2%)	43	72
24	SC	228/356 (64%)	222 (97%)	6 (3%)	40	70
25	SD	272/439 (62%)	258 (95%)	14 (5%)	21	48
27	SJ	234/341 (69%)	224 (96%)	10 (4%)	26	54
28	SK	76/145 (52%)	74 (97%)	2 (3%)	40	70
29	SL	182/413 (44%)	176 (97%)	6 (3%)	33	63
30	SN	156/160 (98%)	152 (97%)	4 (3%)	40	70
31	SO	360/511 (70%)	351 (98%)	9 (2%)	42	71
32	SP	73/233 (31%)	70 (96%)	3 (4%)	27	56
33	SQ	89/126 (71%)	87 (98%)	2 (2%)	45	74
34	SS	158/238 (66%)	146 (92%)	12 (8%)	12	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	ST	383/398 (96%)	364 (95%)	19 (5%)	22	48
35	SU	113/398 (28%)	110 (97%)	3 (3%)	39	69
35	SV	113/398 (28%)	108 (96%)	5 (4%)	25	53
35	SW	105/398 (26%)	101 (96%)	4 (4%)	29	58
36	TN	40/953 (4%)	40 (100%)	0	100	100
38	62	101/151 (67%)	96 (95%)	5 (5%)	22	48
39	63	70/113 (62%)	66 (94%)	4 (6%)	18	43
40	64	72/98 (74%)	69 (96%)	3 (4%)	26	55
41	65	98/122 (80%)	90 (92%)	8 (8%)	10	27
42	66	59/64 (92%)	53 (90%)	6 (10%)	7	18
43	67	77/77 (100%)	73 (95%)	4 (5%)	21	47
44	68	86/109 (79%)	79 (92%)	7 (8%)	11	27
46	24	88/88 (100%)	88 (100%)	0	100	100
46	51	86/88 (98%)	85 (99%)	1 (1%)	63	84
47	25	73/94 (78%)	73 (100%)	0	100	100
47	52	80/94 (85%)	76 (95%)	4 (5%)	22	48
48	2C	100/108 (93%)	97 (97%)	3 (3%)	36	66
49	2D	88/126 (70%)	87 (99%)	1 (1%)	65	85
50	2H	74/79 (94%)	73 (99%)	1 (1%)	59	82
50	5E	71/79 (90%)	68 (96%)	3 (4%)	26	55
51	2I	65/65 (100%)	63 (97%)	2 (3%)	35	65
51	5F	65/65 (100%)	64 (98%)	1 (2%)	57	81
52	2J	64/68 (94%)	64 (100%)	0	100	100
52	5G	64/68 (94%)	62 (97%)	2 (3%)	35	65
53	53	86/93 (92%)	86 (100%)	0	100	100
54	5B	82/90 (91%)	79 (96%)	3 (4%)	30	59
All	All	12121/17274 (70%)	11682 (96%)	439 (4%)	32	60

All (439) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L7	102	GLN
1	L7	105	CYS

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Mol	Chain	Res	Type
1	L7	119	CYS
1	L7	142	THR
1	L7	151	ARG
1	L7	190	LEU
1	L7	221	ARG
1	L7	236	VAL
1	L7	257	HIS
1	L7	315	TRP
3	L9	42	ILE
3	L9	59	ASP
3	L9	77	LYS
3	L9	116	VAL
3	L9	155	ILE
4	LA	73	LYS
4	LA	93	CYS
4	LA	100	ILE
4	LA	108	LEU
4	LA	123	VAL
4	LA	139	THR
4	LA	222	LEU
4	LA	233	ARG
4	LA	294	ILE
4	LA	303	ASP
4	LA	358	VAL
4	LA	360	ASN
4	LA	369	THR
4	LA	452	GLU
4	LA	475	LEU
4	LA	476	THR
4	LA	482	LYS
4	LA	578	ILE
4	LA	606[A]	MET
4	LA	606[B]	MET
4	LA	664	ARG
4	LA	709	GLN
4	LA	738	ARG
4	LA	809	SER
4	LA	841	LEU
4	LA	846	LEU
4	LA	901	LEU
4	LA	929	GLN
4	LA	1147	LEU

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Mol	Chain	Res	Type
4	LA	1206	GLU
4	LA	1259	LEU
4	LA	1348	GLU
4	LA	1353	THR
4	LA	1370	ARG
4	LA	1411	ASP
4	LA	1431	ASN
4	LA	1442	GLN
4	LA	1450	GLU
4	LA	1501	LEU
4	LA	1576	GLU
4	LA	1667	LEU
4	LA	1692	LYS
4	LA	1693	SER
4	LA	1706	VAL
4	LA	1721	SER
4	LA	1855	VAL
4	LA	1863	THR
4	LA	1924	LEU
4	LA	1934	SER
4	LA	1952	VAL
4	LA	1953	LEU
4	LA	1954	ASP
4	LA	2113	ARG
6	LC	8	TYR
6	LC	105	GLU
6	LC	160	VAL
6	LC	201	LEU
6	LC	213	THR
6	LC	217	VAL
6	LC	246	VAL
6	LC	252	LEU
6	LC	256	SER
6	LC	264	ILE
6	LC	285	ILE
6	LC	322	GLU
6	LC	384	THR
6	LC	447	LEU
6	LC	545	LEU
6	LC	588	THR
6	LC	594	LEU
6	LC	605	VAL

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Mol	Chain	Res	Type
6	LC	651	VAL
6	LC	672	LEU
6	LC	678	LEU
6	LC	691	SER
6	LC	745	VAL
6	LC	768	PHE
6	LC	779	ARG
6	LC	781	LEU
6	LC	824	TYR
6	LC	879	THR
6	LC	900	GLU
6	LC	903	CYS
6	LC	934	ILE
6	LC	944	ASP
7	LD	20	THR
7	LD	70	GLU
8	LF	40	GLN
8	LF	50	LEU
8	LF	64	SER
8	LF	93	ARG
8	LF	94	LEU
8	LF	106	VAL
8	LF	111	LEU
8	LF	118	SER
8	LF	256	LEU
8	LF	272	LEU
8	LF	273	LEU
8	LF	390	SER
8	LF	392	CYS
8	LF	447	LEU
8	LF	480	GLN
8	LF	485	GLU
8	LF	592	VAL
8	LF	624	LEU
8	LF	632	THR
8	LF	642	ILE
8	LF	645	THR
8	LF	685	ILE
8	LF	705	ARG
9	LG	6	ARG
10	LH	90	LYS
11	LJ	9	LEU

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Mol	Chain	Res	Type
11	LJ	28	VAL
11	LJ	33	VAL
11	LJ	70	THR
11	LJ	144	VAL
11	LJ	155	LEU
11	LJ	164	GLU
11	LJ	177	LYS
11	LJ	195	GLU
11	LJ	209	ILE
11	LJ	275	CYS
11	LJ	284	VAL
11	LJ	285	VAL
11	LJ	286	ILE
11	LJ	317	SER
11	LJ	376	GLU
11	LJ	389	THR
11	LJ	397	HIS
11	LJ	435	VAL
11	LJ	451	GLN
12	LL	100	ARG
12	LL	101	HIS
12	LL	199	ARG
13	LN	8	SER
13	LN	28	ASP
13	LN	49	LEU
13	LN	59	GLU
13	LN	61	VAL
13	LN	62	CYS
13	LN	107	ARG
13	LN	110	VAL
13	LN	125	THR
13	LN	131	VAL
13	LN	143	ASP
13	LN	149	VAL
13	LN	157	VAL
13	LN	163	THR
13	LN	178	LEU
13	LN	195	CYS
13	LN	213	VAL
13	LN	241	ARG
13	LN	262	THR
13	LN	264	VAL

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Mol	Chain	Res	Type
13	LN	267	ASN
13	LN	285	THR
13	LN	287	THR
13	LN	310	CYS
13	LN	317	VAL
14	LP	11	GLU
14	LP	16	GLN
14	LP	162	LEU
15	LQ	29	ARG
15	LQ	94	THR
15	LQ	120	LEU
15	LQ	163	SER
15	LQ	167	THR
15	LQ	171	GLU
15	LQ	194	LEU
15	LQ	215	ARG
15	LQ	223	LEU
15	LQ	235	LEU
15	LQ	286	VAL
15	LQ	642	ARG
15	LQ	697	LEU
15	LQ	701	ASP
15	LQ	715	LEU
15	LQ	755	LEU
16	LR	161	GLN
17	LS	36	VAL
17	LS	61	VAL
17	LS	64	HIS
17	LS	84	VAL
17	LS	152	VAL
17	LS	163	VAL
17	LS	215	ILE
17	LS	220	VAL
17	LS	262	ILE
17	LS	267	GLU
17	LS	352	LEU
17	LS	353	THR
17	LS	422	GLN
17	LS	443	LEU
17	LS	462	CYS
17	LS	478	ASP
17	LS	497	CYS

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Mol	Chain	Res	Type
17	LS	498	LEU
17	LS	504	GLN
17	LS	617	HIS
17	LS	680	TYR
17	LS	689	THR
17	LS	764	THR
17	LS	767	THR
17	LS	785	SER
17	LS	787	LEU
18	LT	14	VAL
18	LT	87	GLN
18	LT	121	ARG
18	LT	125	THR
18	LT	171	SER
18	LT	285	LEU
18	LT	326	ASP
18	LT	489	ARG
18	LT	524	CYS
18	LT	532	THR
18	LT	608	LEU
18	LT	652	THR
18	LT	661	SER
18	LT	696	ASP
18	LT	698	VAL
18	LT	715	LEU
19	LV	52	THR
19	LV	128	LEU
19	LV	141	VAL
19	LV	219	LEU
19	LV	223	ARG
19	LV	525	LEU
19	LV	559	VAL
19	LV	573	VAL
19	LV	574	THR
19	LV	594	ARG
19	LV	607	LEU
19	LV	639	THR
19	LV	666	LEU
19	LV	710	ILE
19	LV	730	LYS
19	LV	742	SER
19	LV	766	THR

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Mol	Chain	Res	Type
19	LV	767	GLU
19	LV	790	VAL
19	LV	983	VAL
19	LV	986	HIS
19	LV	1008	ILE
19	LV	1016	LEU
19	LV	1034	ILE
19	LV	1056	THR
19	LV	1073	THR
20	LW	58	LEU
20	LW	63	THR
20	LW	139	VAL
20	LW	165	LEU
21	LY	18	SER
21	LY	23	ARG
21	LY	94	GLU
21	LY	98	ARG
23	SA	145	VAL
23	SA	193	LEU
23	SA	217	LEU
23	SA	221	LEU
23	SA	262	THR
23	SA	267	ASP
23	SA	360	ARG
23	SA	364	LEU
23	SA	442	THR
23	SA	462	VAL
23	SA	533	LEU
24	SC	24	LEU
24	SC	67	LEU
24	SC	154	ARG
24	SC	159	VAL
24	SC	195	ARG
24	SC	293	GLN
25	SD	6	LEU
25	SD	243	LEU
25	SD	313	VAL
25	SD	343	GLN
25	SD	477	LYS
25	SD	480	LEU
25	SD	489	ARG
25	SD	493	GLU

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Mol	Chain	Res	Type
25	SD	505	ASN
25	SD	513	LEU
25	SD	517	ARG
25	SD	526	ASN
25	SD	528	LEU
25	SD	536	CYS
27	SJ	90	VAL
27	SJ	143	LEU
27	SJ	152	THR
27	SJ	153	LEU
27	SJ	223	SER
27	SJ	224	ARG
27	SJ	238	THR
27	SJ	264	LEU
27	SJ	269	VAL
27	SJ	361	LEU
28	SK	53	VAL
28	SK	138	VAL
29	SL	3	LEU
29	SL	13	ASP
29	SL	141	LEU
29	SL	256	THR
29	SL	271	LYS
29	SL	306	GLN
30	SN	42	LEU
30	SN	106	ILE
30	SN	156	SER
30	SN	173	VAL
31	SO	289	VAL
31	SO	376	GLU
31	SO	411	GLU
31	SO	419	LEU
31	SO	442	VAL
31	SO	449	TYR
31	SO	481	LEU
31	SO	504	THR
31	SO	550	SER
32	SP	201	LEU
32	SP	228	LEU
32	SP	250	LEU
33	SQ	1	MET
33	SQ	18	THR

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Mol	Chain	Res	Type
34	SS	35	LEU
34	SS	41	THR
34	SS	100	TYR
34	SS	102	CYS
34	SS	106	ASP
34	SS	117	LEU
34	SS	183	GLN
34	SS	204	LEU
34	SS	208	GLN
34	SS	217	GLU
34	SS	256	LEU
34	SS	262	VAL
35	ST	4	CYS
35	ST	77	LEU
35	ST	101	GLN
35	ST	127	LEU
35	ST	187	THR
35	ST	209	VAL
35	ST	211	LEU
35	ST	216	GLU
35	ST	296	VAL
35	ST	309	ILE
35	ST	330	VAL
35	ST	335	LEU
35	ST	336	THR
35	ST	347	VAL
35	ST	348	GLU
35	ST	419	GLN
35	ST	479	THR
35	ST	485	VAL
35	ST	496	CYS
35	SU	64	VAL
35	SU	69	LEU
35	SU	82	GLN
35	SV	74	VAL
35	SV	76	THR
35	SV	77	LEU
35	SV	84	GLU
35	SV	106	LEU
35	SW	53	THR
35	SW	81	LEU
35	SW	102	LEU

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Mol	Chain	Res	Type
35	SW	106	LEU
38	62	69	THR
38	62	81	LEU
38	62	87	VAL
38	62	100	LEU
38	62	123	CYS
39	63	41	HIS
39	63	63	CYS
39	63	67	LEU
39	63	117	SER
40	64	17	CYS
40	64	23	SER
40	64	39	THR
41	65	12	GLN
41	65	34	ILE
41	65	46	ARG
41	65	58	GLU
41	65	78	VAL
41	65	82	THR
41	65	130	CYS
41	65	147	LEU
42	66	5	LEU
42	66	13	VAL
42	66	21	GLU
42	66	36	VAL
42	66	58	LEU
42	66	62	ASN
43	67	8	VAL
43	67	18	LEU
43	67	46	VAL
43	67	91	ILE
44	68	15	VAL
44	68	31	LEU
44	68	42	ILE
44	68	81	LEU
44	68	99	ILE
44	68	101	VAL
44	68	102	ILE
48	2C	46	CYS
48	2C	54	VAL
48	2C	84	ARG
49	2D	53	VAL

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Mol	Chain	Res	Type
50	2H	50	VAL
51	2I	36	ASP
51	2I	61	LEU
46	51	43	ASP
47	52	42	VAL
47	52	46	CYS
47	52	80	GLU
47	52	89	VAL
54	5B	43	VAL
54	5B	66	ILE
54	5B	77	THR
50	5E	30	VAL
50	5E	50	VAL
50	5E	55	THR
51	5F	5	VAL
52	5G	22	ILE
52	5G	58	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
1	L7	102	GLN
1	L7	305	HIS
3	L9	102	GLN
3	L9	156	HIS
4	LA	315	HIS
4	LA	639	GLN
4	LA	915	HIS
4	LA	1004	ASN
4	LA	1242	ASN
4	LA	1329	HIS
4	LA	1498	HIS
4	LA	1532	HIS
4	LA	1622	GLN
4	LA	1660	HIS
4	LA	1686	GLN
4	LA	1945	GLN
4	LA	2024	ASN
6	LC	95	GLN
6	LC	184	HIS
6	LC	255	HIS
6	LC	910	GLN

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Mol	Chain	Res	Type
8	LF	89	ASN
11	LJ	306	HIS
13	LN	209	HIS
14	LP	190	ASN
15	LQ	89	GLN
15	LQ	123	GLN
15	LQ	280	GLN
15	LQ	700	GLN
15	LQ	703	HIS
15	LQ	706	HIS
15	LQ	714	GLN
15	LQ	798	HIS
16	LR	25	ASN
17	LS	255	GLN
17	LS	293	ASN
18	LT	193	ASN
18	LT	359	ASN
18	LT	509	HIS
18	LT	515	HIS
18	LT	752	HIS
19	LV	42	GLN
19	LV	109	ASN
19	LV	789	HIS
19	LV	932	HIS
19	LV	953	ASN
20	LW	36	HIS
20	LW	103	ASN
20	LW	106	HIS
20	LW	143	ASN
23	SA	8	HIS
23	SA	189	HIS
25	SD	15	GLN
25	SD	296	HIS
25	SD	370	HIS
27	SJ	33	GLN
29	SL	21	HIS
30	SN	118	HIS
30	SN	129	HIS
30	SN	138	GLN
31	SO	405	HIS
33	SQ	73	ASN
34	SS	183	GLN

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Mol	Chain	Res	Type
35	ST	167	HIS
35	ST	231	HIS
35	ST	255	HIS
35	ST	361	GLN
35	SU	92	GLN
35	SU	97	GLN
35	SU	98	GLN
38	62	82	HIS
39	63	43	HIS
40	64	33	ASN
41	65	64	GLN
41	65	132	GLN
42	66	11	GLN
43	67	33	HIS
43	67	36	HIS
43	67	76	ASN
44	68	25	HIS
47	25	30	ASN
47	25	62	HIS
50	2H	31	HIS
50	2H	34	GLN
51	2I	65	ASN
52	2J	38	HIS
52	2J	44	HIS
54	5B	23	ASN
54	5B	48	GLN
54	5B	72	HIS
50	5E	31	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
45	RN	1/68 (1%)	1 (100%)	0
55	LE	23/39 (58%)	3 (13%)	0
56	LO	45/57 (78%)	5 (11%)	1 (2%)
57	N2	73/142 (51%)	10 (13%)	0
58	N5	61/71 (85%)	8 (13%)	0
59	N6	99/100 (99%)	10 (10%)	1 (1%)
All	All	302/477 (63%)	37 (12%)	2 (0%)

All (37) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
45	RN	44	G
55	LE	16	A
55	LE	22	A
55	LE	23	G
56	LO	73	A
56	LO	74	G
56	LO	80	G
56	LO	81	G
56	LO	82	A
57	N2	7	U
57	N2	15	A
57	N2	17	U
57	N2	18	U
57	N2	20	G
57	N2	24	A
57	N2	25	G
57	N2	92	U
57	N2	94	A
57	N2	128	U
58	N5	5	C
58	N5	17	U
58	N5	22	C
58	N5	56	G
58	N5	57	A
58	N5	65	A
58	N5	66	A
58	N5	67	G
59	N6	3	A
59	N6	10	U
59	N6	11	C
59	N6	26	A
59	N6	44	G
59	N6	47	G
59	N6	60	C
59	N6	66	C
59	N6	72	U
59	N6	100	U

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
56	LO	81	G
59	N6	9	U

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	SEP	SL	186	29	8,9,10	1.47	1 (12%)	8,12,14	1.16	1 (12%)
55	PSU	LE	28	55	18,21,22	1.06	1 (5%)	22,30,33	1.81	4 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	SEP	SL	186	29	-	0/5/8/10	-
55	PSU	LE	28	55	-	1/7/25/26	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	LE	28	PSU	C6-C5	3.32	1.39	1.35
29	SL	186	SEP	P-O1P	3.20	1.60	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	LE	28	PSU	C4-N3-C2	-4.66	119.63	126.34
55	LE	28	PSU	N1-C2-N3	4.58	120.32	115.13
55	LE	28	PSU	O2-C2-N1	-2.84	119.67	122.79
55	LE	28	PSU	C6-N1-C2	-2.29	120.34	122.68
29	SL	186	SEP	P-OG-CB	-2.28	112.02	118.30

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	LE	28	PSU	O4'-C1'-C5-C4

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 18 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
61	ADP	L7	702	62,60	27,29,29	1.30	4 (14%)	42,45,45	1.97	10 (23%)
66	GTG	N5	101	58	53,57,57	3.45	20 (37%)	79,90,90	2.91	33 (41%)
67	G5J	N6	201	59	31,35,35	0.74	1 (3%)	38,55,55	0.92	2 (5%)
63	IHP	LA	2501	-	36,36,36	1.44	6 (16%)	54,60,60	0.98	3 (5%)
64	GTP	LC	1500	60	30,34,34	2.98	14 (46%)	46,54,54	1.93	15 (32%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	ADP	L7	702	62,60	-	4/16/32/32	0/3/3/3
66	GTG	N5	101	58	-	8/32/64/64	0/6/6/6
67	G5J	N6	201	59	-	5/25/41/41	0/3/3/3
63	IHP	LA	2501	-	-	2/30/54/54	0/1/1/1
64	GTP	LC	1500	60	-	3/22/38/38	0/3/3/3

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	N5	101	GTG	O3D-C3D	-10.17	1.19	1.43
66	N5	101	GTG	O6B-C6B	8.59	1.39	1.23
66	N5	101	GTG	O6A-C6A	8.56	1.39	1.23
64	LC	1500	GTP	O6-C6	8.55	1.39	1.23
66	N5	101	GTG	C5A-N7A	8.10	1.48	1.39
64	LC	1500	GTP	C5-N7	6.82	1.52	1.39
66	N5	101	GTG	C5B-N7B	6.64	1.52	1.39
66	N5	101	GTG	C5A-C4A	6.33	1.54	1.38
66	N5	101	GTG	C2A-N2A	4.75	1.45	1.34
64	LC	1500	GTP	C2-N2	4.60	1.45	1.34
66	N5	101	GTG	C2B-N2B	4.58	1.45	1.34
64	LC	1500	GTP	C2-N1	4.39	1.48	1.37
66	N5	101	GTG	O4E-C1E	4.34	1.52	1.42
64	LC	1500	GTP	C8-N9	-4.29	1.27	1.37
64	LC	1500	GTP	C2-N3	4.23	1.43	1.33
66	N5	101	GTG	C4B-N9B	-4.06	1.27	1.38
61	L7	702	ADP	C5-C4	4.04	1.46	1.39
66	N5	101	GTG	C8B-N9B	-3.91	1.28	1.37
66	N5	101	GTG	C4A-N9A	3.68	1.47	1.38
64	LC	1500	GTP	C4-N9	-3.59	1.28	1.38
66	N5	101	GTG	C2A-N1A	3.36	1.46	1.37
66	N5	101	GTG	C2E-C3E	-3.34	1.44	1.53
66	N5	101	GTG	O4E-C4E	3.25	1.52	1.45
63	LA	2501	IHP	P5-O15	3.07	1.65	1.59
63	LA	2501	IHP	P4-O14	3.05	1.65	1.59
63	LA	2501	IHP	P6-O16	2.97	1.64	1.59
63	LA	2501	IHP	P2-O12	2.84	1.64	1.59
63	LA	2501	IHP	P1-O11	2.80	1.64	1.59
63	LA	2501	IHP	P3-O13	2.76	1.64	1.59
66	N5	101	GTG	C2D-C3D	-2.75	1.45	1.53
67	N6	201	G5J	C6-C5	-2.50	1.37	1.45
61	L7	702	ADP	C5-N7	-2.49	1.34	1.39
64	LC	1500	GTP	O4'-C1'	2.41	1.47	1.42
64	LC	1500	GTP	PG-O3G	-2.41	1.45	1.54
64	LC	1500	GTP	PG-O2G	-2.39	1.45	1.54
66	N5	101	GTG	C4B-N3B	2.36	1.39	1.34
66	N5	101	GTG	C5B-C4B	2.36	1.45	1.38
61	L7	702	ADP	C5-C6	2.32	1.47	1.41
64	LC	1500	GTP	C4-N3	2.29	1.39	1.34
64	LC	1500	GTP	C2'-C3'	-2.22	1.47	1.53
61	L7	702	ADP	C8-N7	2.20	1.35	1.31
64	LC	1500	GTP	PA-O2A	-2.11	1.45	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	LC	1500	GTP	PB-O2B	-2.09	1.45	1.55
66	N5	101	GTG	C2A-N3A	2.08	1.38	1.33
66	N5	101	GTG	C8B-N7B	2.05	1.38	1.32

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	N5	101	GTG	C8A-N7A-C5A	8.78	118.76	107.78
66	N5	101	GTG	C6A-C5A-N7A	8.60	142.65	132.25
66	N5	101	GTG	C8B-N9B-C4B	7.57	120.46	106.05
66	N5	101	GTG	N9A-C4A-N3A	7.14	140.27	125.94
64	LC	1500	GTP	C8-N9-C4	6.85	119.09	106.05
61	L7	702	ADP	C5-C4-N3	-6.21	118.64	126.75
66	N5	101	GTG	C5B-C4B-N3B	-5.30	119.86	128.46
66	N5	101	GTG	N9B-C4B-N3B	5.24	136.46	125.94
66	N5	101	GTG	C2A-N3A-C4A	4.99	121.19	112.30
61	L7	702	ADP	N3-C4-N9	4.85	135.07	127.08
66	N5	101	GTG	C4A-C5A-N7A	-4.84	99.76	107.67
66	N5	101	GTG	C7X-N7A-C5A	-4.81	120.80	126.77
66	N5	101	GTG	C5A-C4A-N3A	-4.70	119.14	128.15
66	N5	101	GTG	C8A-N9A-C4A	4.61	118.83	107.16
66	N5	101	GTG	C2B-N3B-C4B	4.45	120.22	112.30
66	N5	101	GTG	N9A-C8A-N7A	-4.10	102.06	112.21
61	L7	702	ADP	C2-N3-C4	4.07	121.37	111.75
66	N5	101	GTG	C6B-C5B-N7B	3.96	137.62	130.25
66	N5	101	GTG	C4B-C5B-N7B	-3.88	104.58	110.72
66	N5	101	GTG	C5A-C6A-N1A	3.83	119.80	111.79
66	N5	101	GTG	O6A-C6A-C5A	-3.69	119.74	128.06
61	L7	702	ADP	N3-C2-N1	-3.56	123.04	128.60
66	N5	101	GTG	N9B-C8B-N7B	-3.30	107.18	113.39
64	LC	1500	GTP	C3'-C2'-C1'	3.26	107.63	101.43
64	LC	1500	GTP	PB-O3B-PG	-3.19	121.87	132.83
61	L7	702	ADP	PA-O3A-PB	-3.18	121.91	132.83
64	LC	1500	GTP	C2-N1-C6	-3.18	119.30	125.10
63	LA	2501	IHP	C6-C1-C2	3.18	117.36	110.41
66	N5	101	GTG	C2B-N1B-C6B	-3.04	119.56	125.10
61	L7	702	ADP	C4-C5-N7	-3.02	106.94	110.62
64	LC	1500	GTP	O3G-PG-O3B	2.98	114.63	104.64
66	N5	101	GTG	PB-O3A-PA	-2.90	122.86	132.83
66	N5	101	GTG	C7X-N7A-C8A	-2.85	120.44	124.84
66	N5	101	GTG	C2A-N1A-C6A	-2.75	120.09	125.10
63	LA	2501	IHP	C3-C2-C1	2.73	116.40	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	L7	702	ADP	C5-N7-C8	2.72	107.38	103.51
66	N5	101	GTG	C5B-C6B-N1B	2.66	119.94	113.19
66	N5	101	GTG	C4E-O4E-C1E	-2.63	103.66	109.47
66	N5	101	GTG	C3D-C2D-C1D	2.62	106.41	101.43
64	LC	1500	GTP	C5-C6-N1	2.59	119.76	113.19
64	LC	1500	GTP	N9-C4-N3	2.55	131.06	125.94
61	L7	702	ADP	C4-N9-C8	2.53	108.47	105.73
66	N5	101	GTG	O6B-C6B-C5B	-2.51	119.93	126.60
64	LC	1500	GTP	O2G-PG-O3B	2.50	113.02	104.64
63	LA	2501	IHP	C6-C5-C4	-2.48	104.97	110.41
64	LC	1500	GTP	C1'-N9-C8	-2.46	119.69	126.70
66	N5	101	GTG	C5A-C4A-N9A	-2.42	100.59	105.89
66	N5	101	GTG	C1E-N9B-C8B	-2.41	119.83	126.70
64	LC	1500	GTP	O2A-PA-O1A	-2.34	100.69	112.24
66	N5	101	GTG	PG-O3B-PB	-2.33	124.82	132.83
66	N5	101	GTG	C1E-N9B-C4B	-2.29	119.71	126.50
64	LC	1500	GTP	O6-C6-C5	-2.27	120.59	126.60
66	N5	101	GTG	O2G-PG-O1G	-2.24	101.16	112.24
64	LC	1500	GTP	C2'-C3'-C4'	2.24	106.99	102.64
61	L7	702	ADP	N9-C8-N7	-2.19	110.92	113.91
61	L7	702	ADP	C6-C5-N7	2.18	136.09	132.02
67	N6	201	G5J	PG-O3B-PB	-2.17	125.37	132.83
66	N5	101	GTG	O2A-PA-O1A	-2.15	101.59	112.24
67	N6	201	G5J	PB-O3A-PA	-2.11	125.59	132.83
64	LC	1500	GTP	O2B-PB-O1B	-2.08	101.93	112.24
64	LC	1500	GTP	C5-C4-N9	-2.06	101.89	105.63
66	N5	101	GTG	O2B-PB-O1B	-2.05	102.11	112.24
64	LC	1500	GTP	C8-N7-C5	-2.02	100.58	104.24

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
61	L7	702	ADP	PA-O3A-PB-O2B
64	LC	1500	GTP	PB-O3B-PG-O2G
64	LC	1500	GTP	PB-O3B-PG-O3G
66	N5	101	GTG	C5D-O5D-PA-O3A
66	N5	101	GTG	PB-O3B-PG-O5E
66	N5	101	GTG	C3E-C4E-C5E-O5E
67	N6	201	G5J	C5'-O5'-PA-O1A
67	N6	201	G5J	C5'-O5'-PA-O2A
66	N5	101	GTG	O4E-C4E-C5E-O5E

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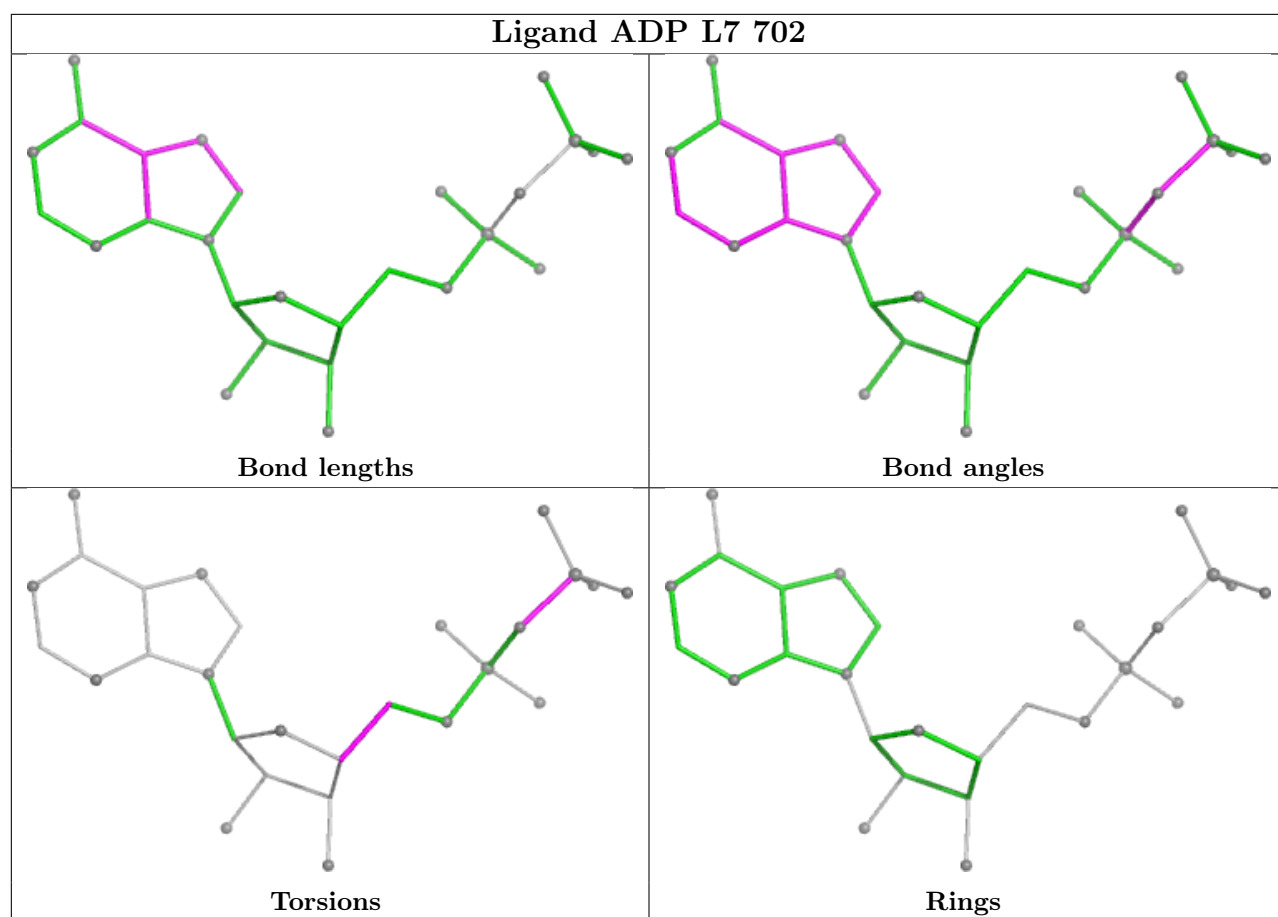
Mol	Chain	Res	Type	Atoms
67	N6	201	G5J	O4'-C1'-N9-C4
67	N6	201	G5J	O4'-C1'-N9-C8
66	N5	101	GTG	C4E-C5E-O5E-PG
61	L7	702	ADP	PA-O3A-PB-O3B
63	LA	2501	IHP	C4-O14-P4-O34
61	L7	702	ADP	O4'-C4'-C5'-O5'
66	N5	101	GTG	C5D-O5D-PA-O2A
61	L7	702	ADP	PA-O3A-PB-O1B
63	LA	2501	IHP	C4-O14-P4-O44
67	N6	201	G5J	C5'-O5'-PA-O3A
66	N5	101	GTG	C4D-C5D-O5D-PA
66	N5	101	GTG	O4D-C4D-C5D-O5D
64	LC	1500	GTP	PA-O3A-PB-O1B

There are no ring outliers.

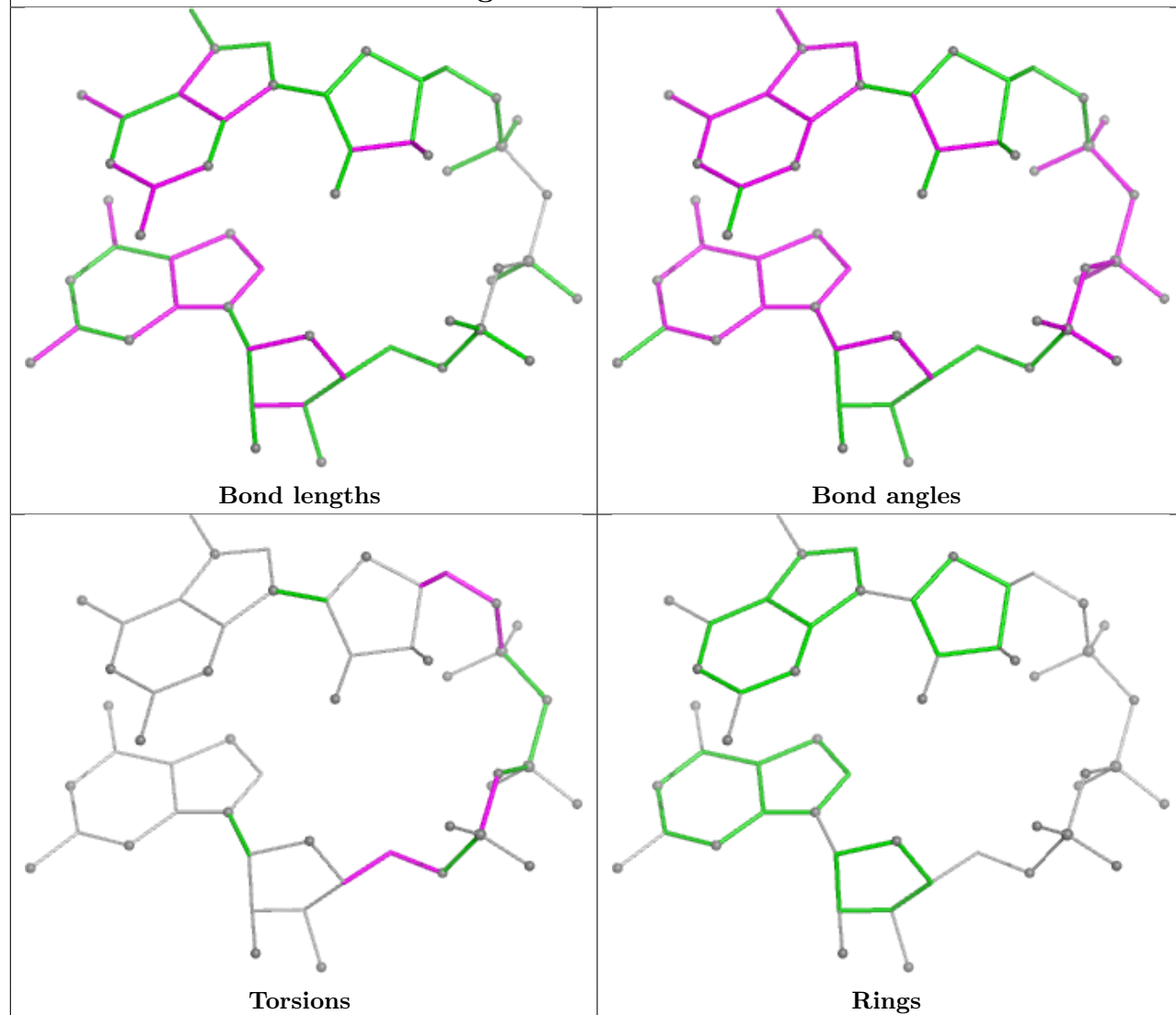
2 monomers are involved in 5 short contacts:

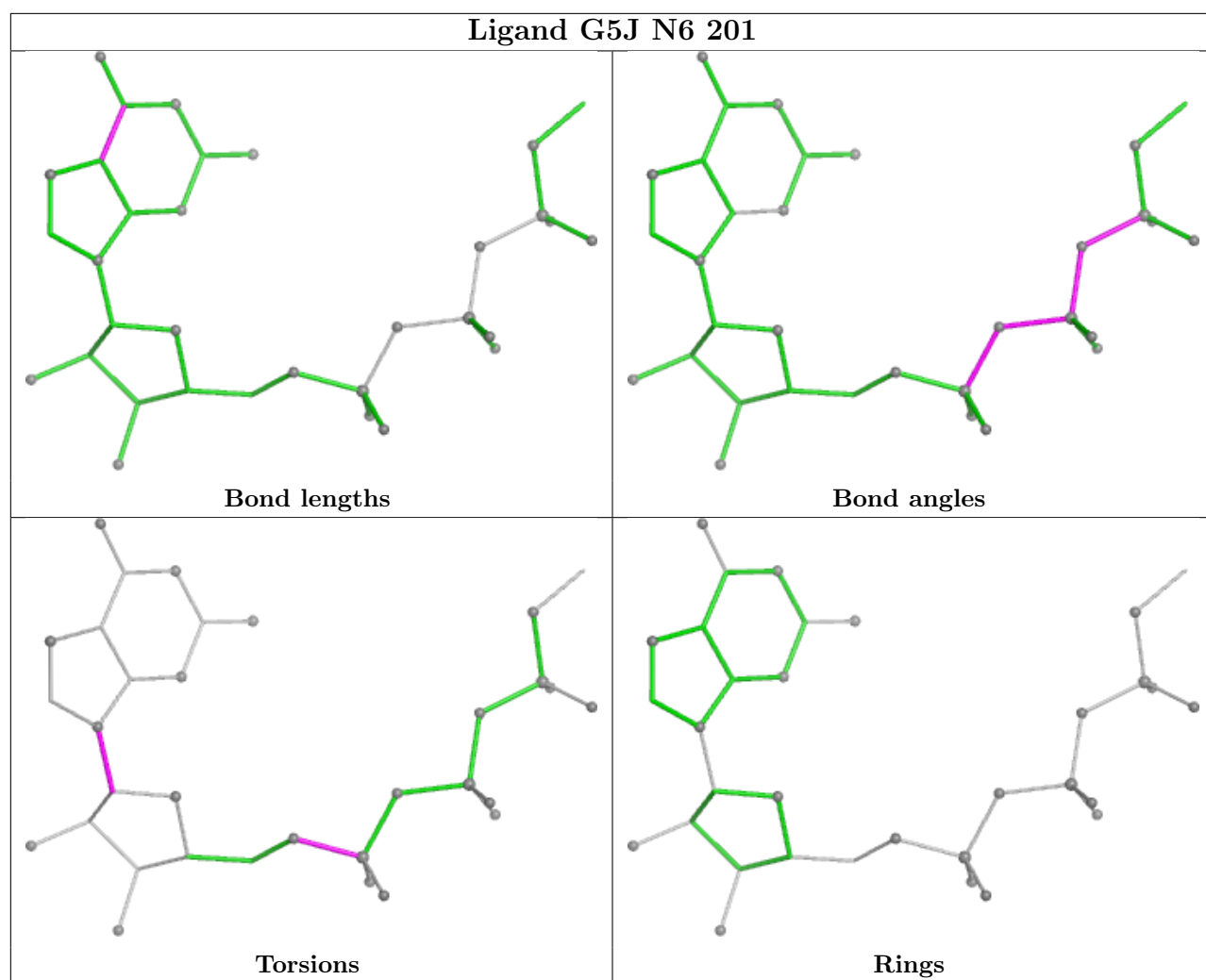
Mol	Chain	Res	Type	Clashes	Symm-Clashes
67	N6	201	G5J	3	0
63	LA	2501	IHP	2	0

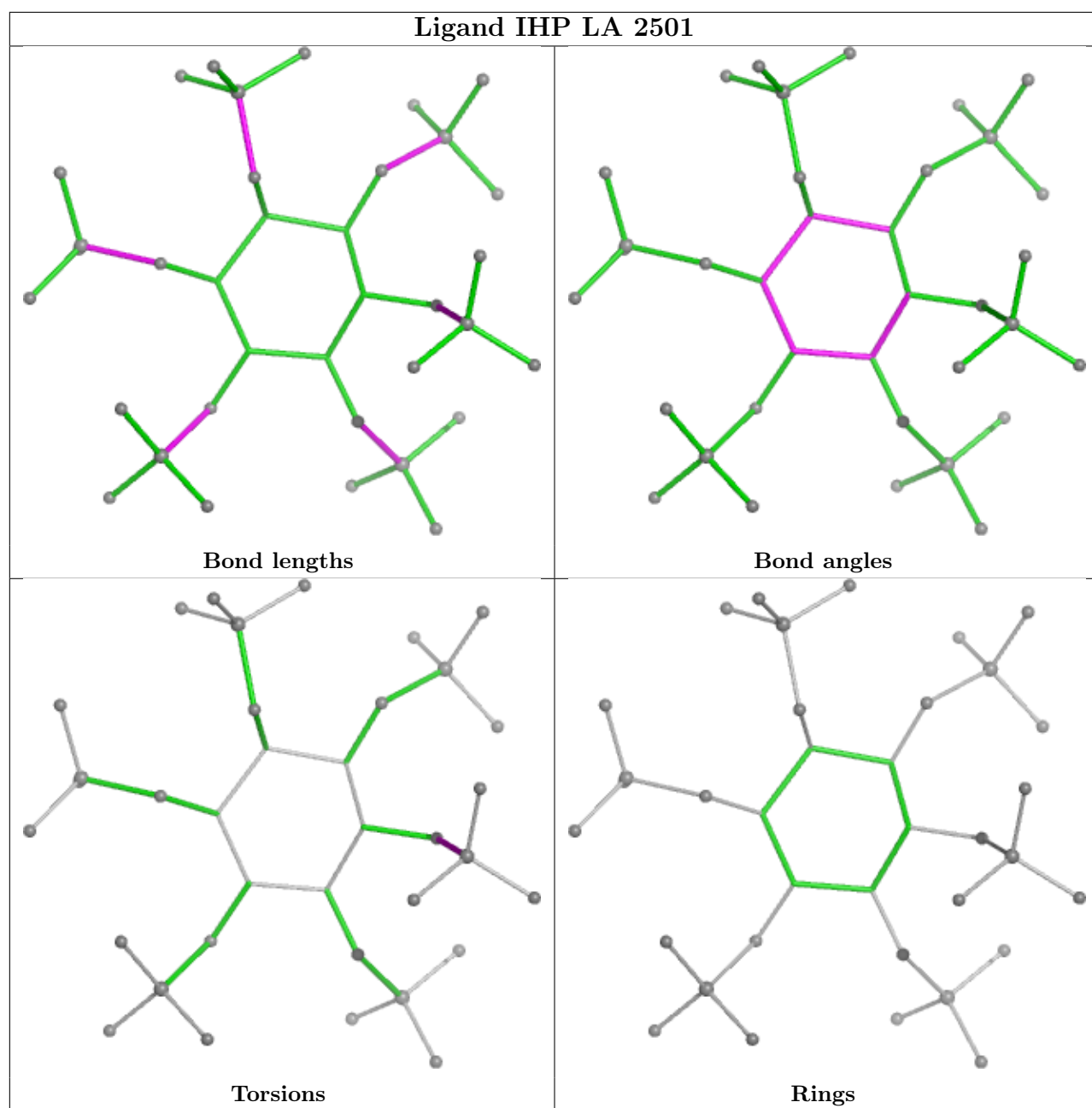
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

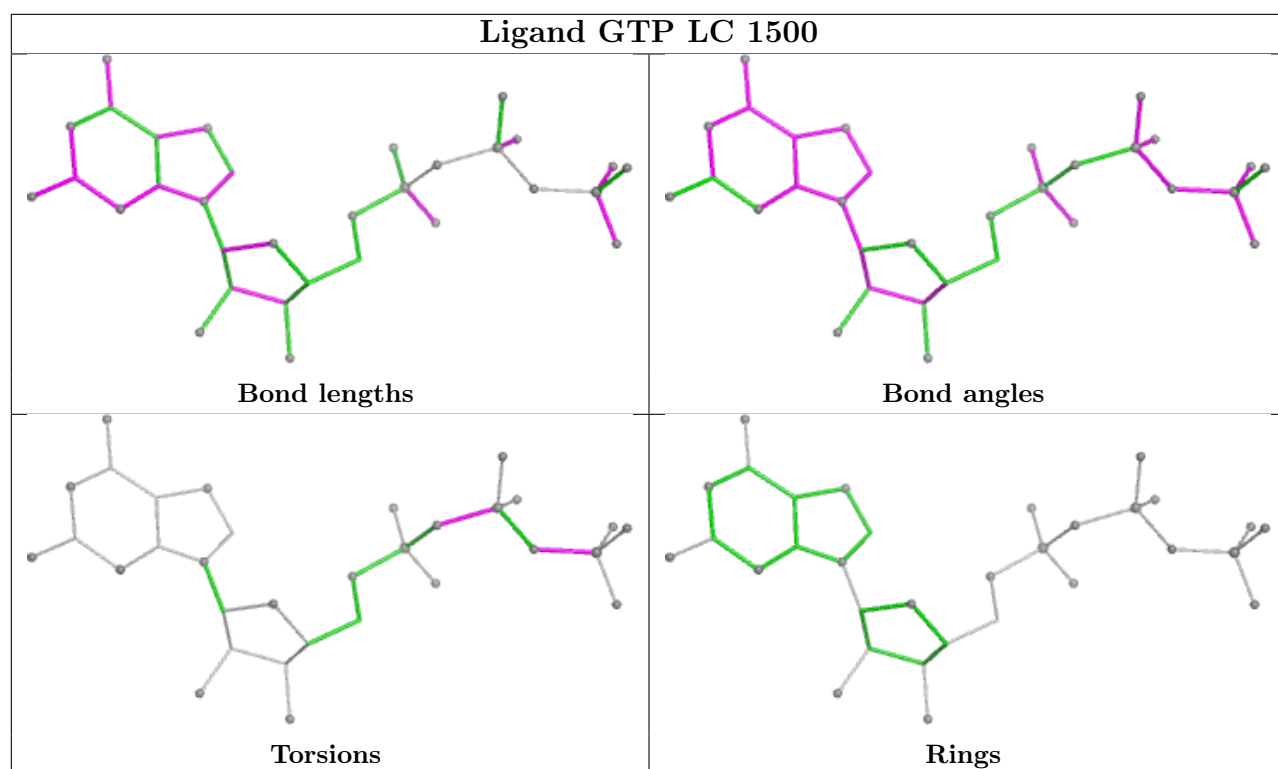


Ligand GTG N5 101









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

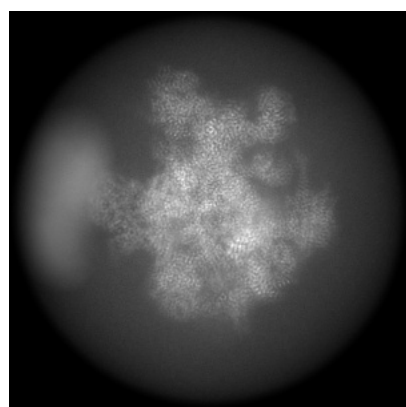
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52843. These allow visual inspection of the internal detail of the map and identification of artifacts.

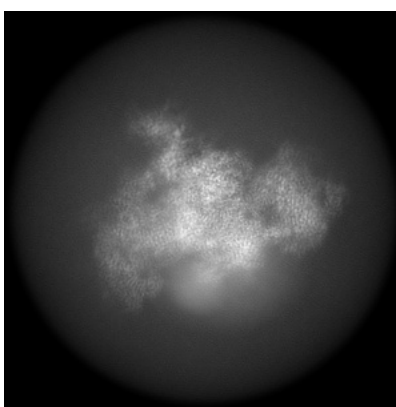
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

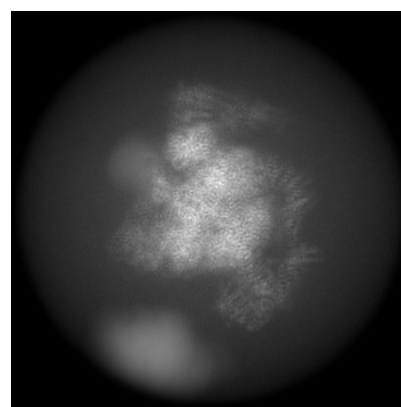
6.1.1 Primary map



X



Y

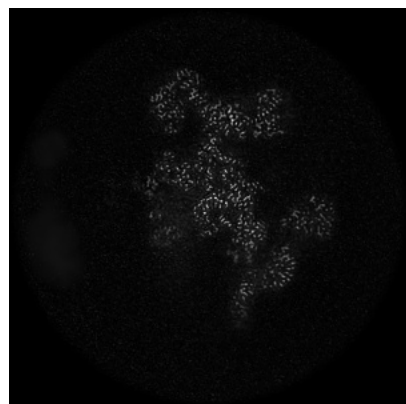


Z

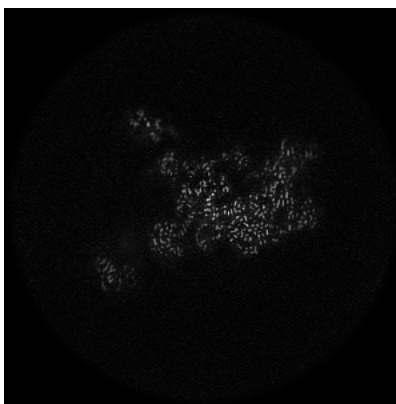
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

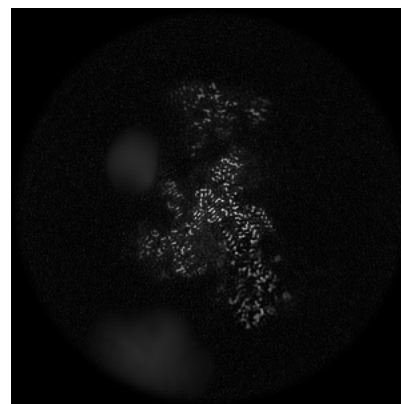
6.2.1 Primary map



X Index: 200



Y Index: 200

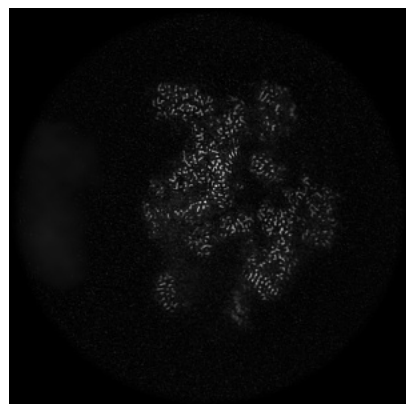


Z Index: 200

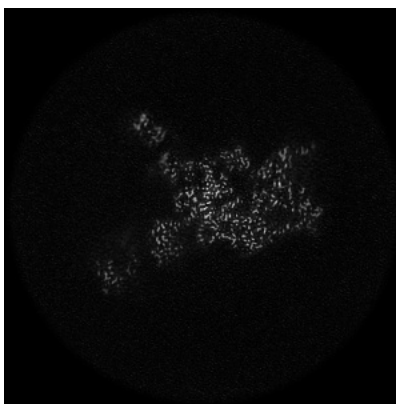
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

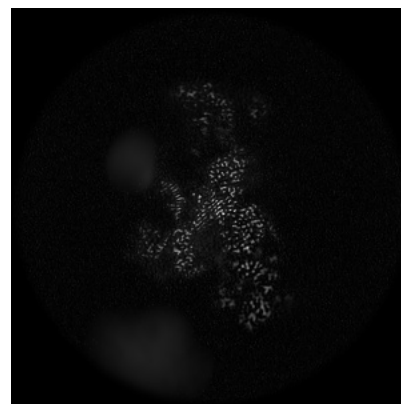
6.3.1 Primary map



X Index: 184



Y Index: 197

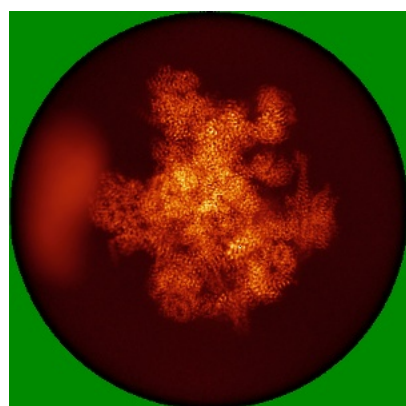


Z Index: 203

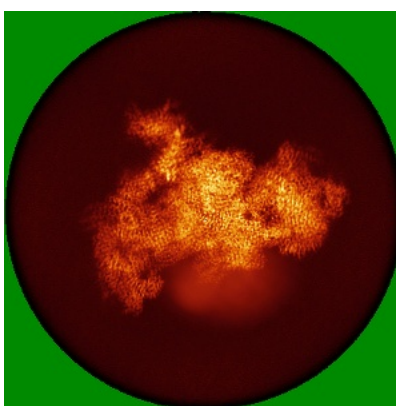
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

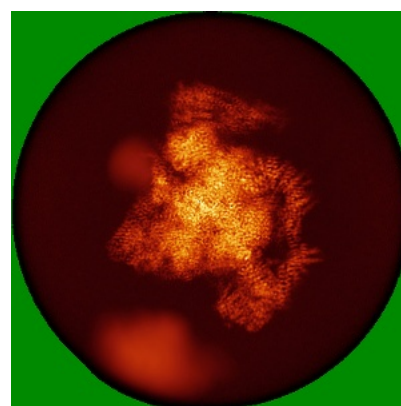
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

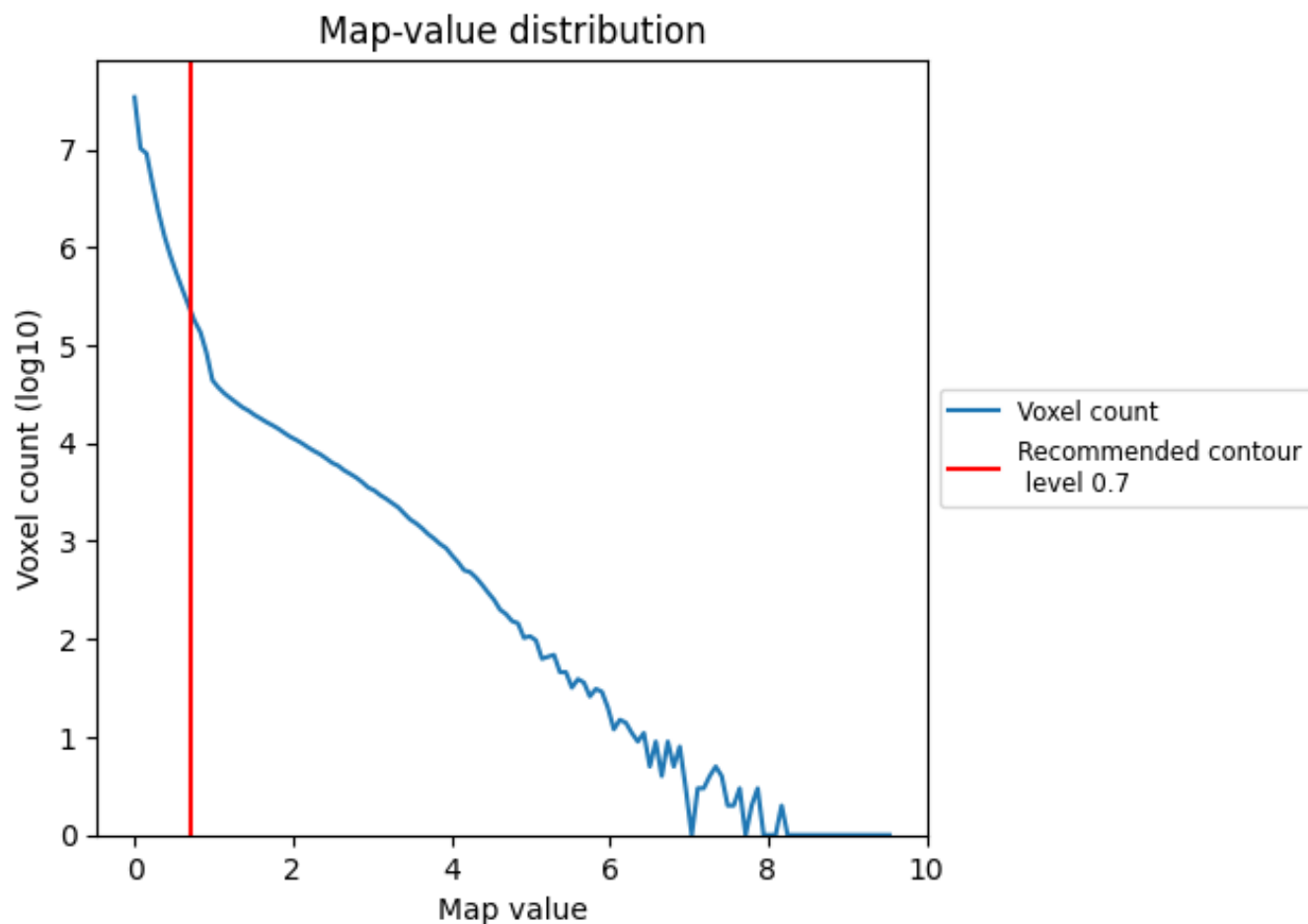
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

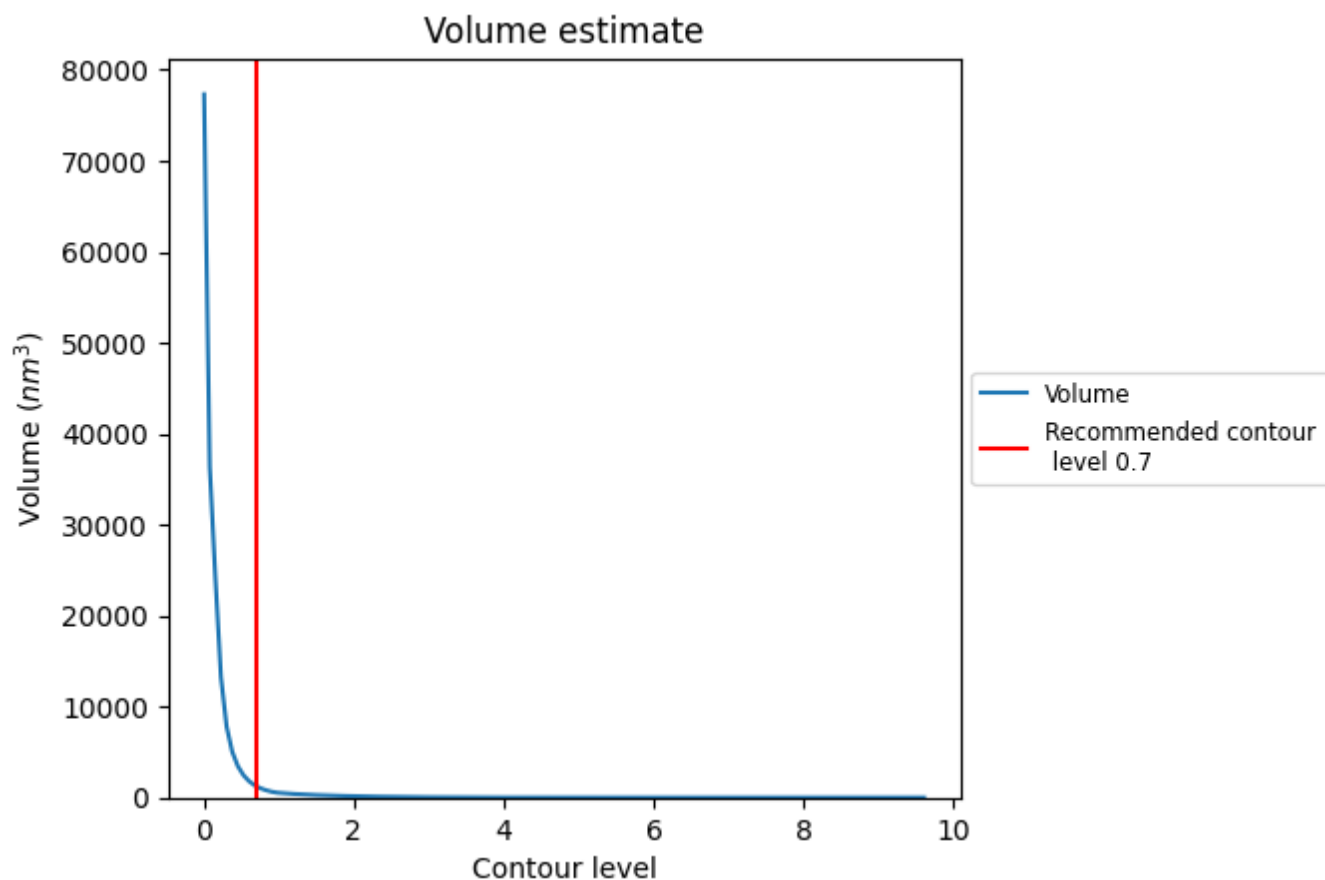
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

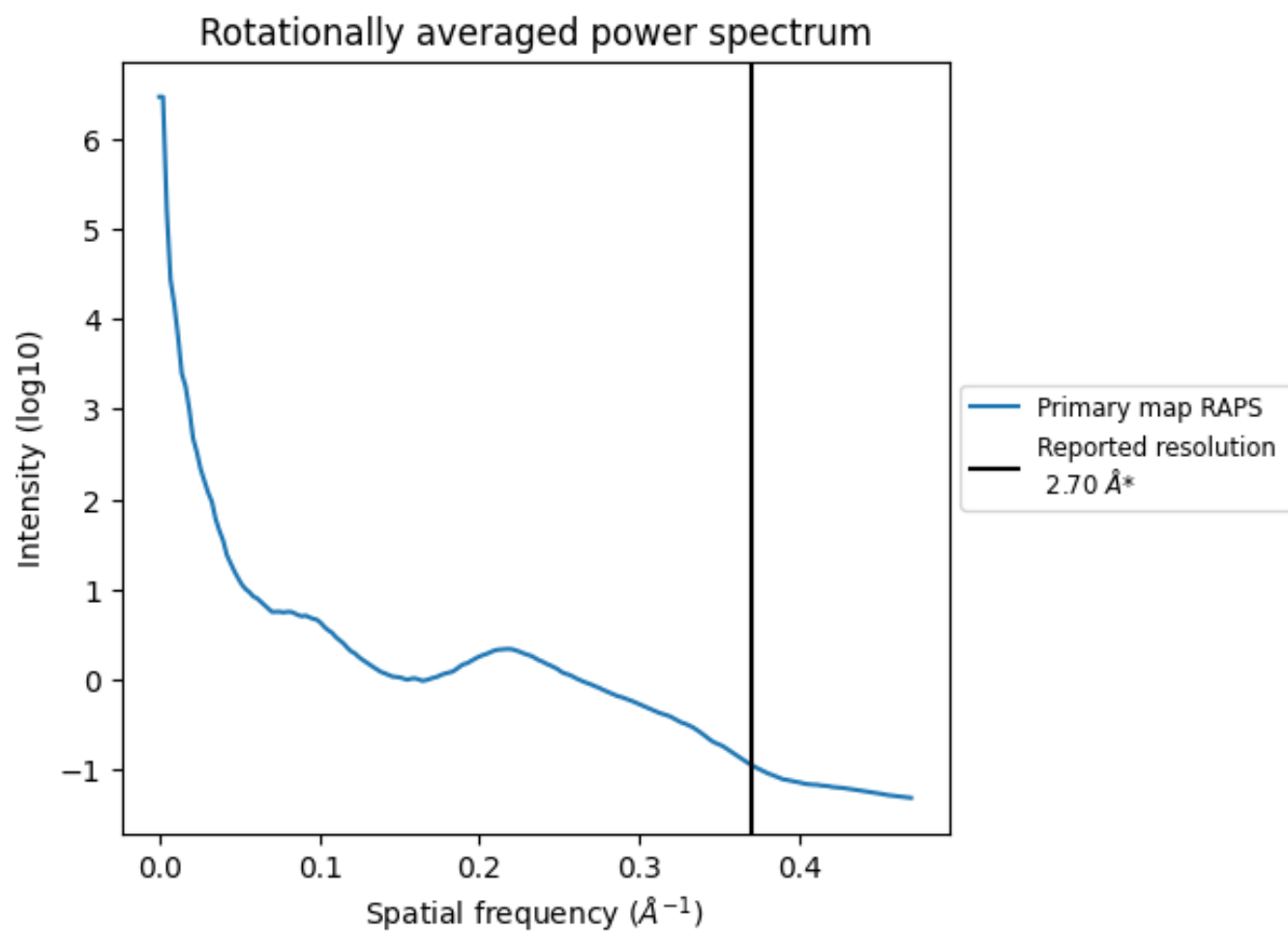
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1240 nm^3 ; this corresponds to an approximate mass of 1120 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

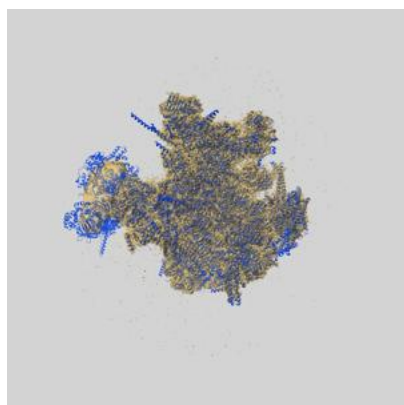
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

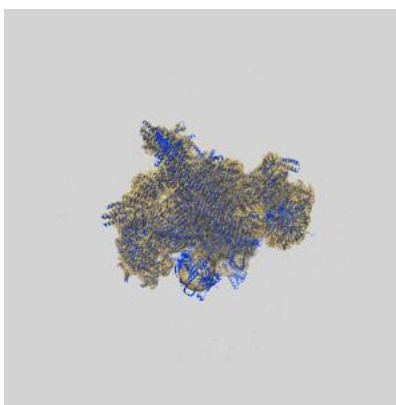
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52843 and PDB model 9IF7. Per-residue inclusion information can be found in section 3 on page 19.

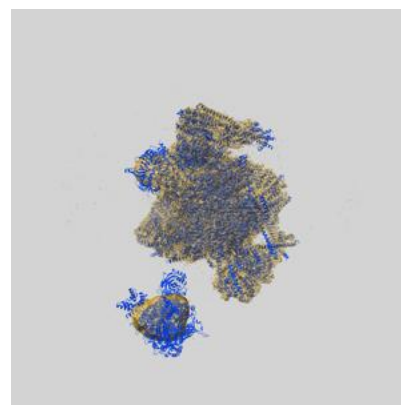
9.1 Map-model overlay [i](#)



X



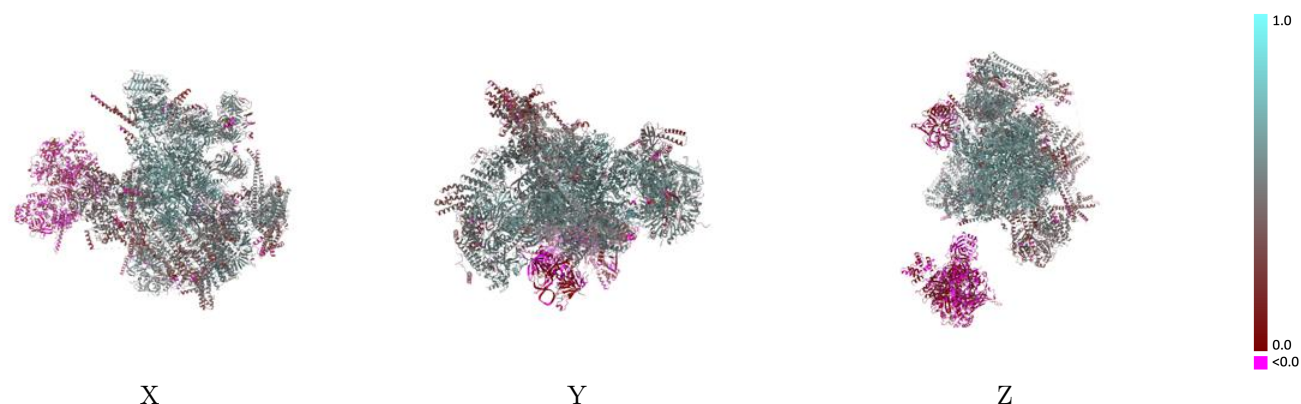
Y



Z

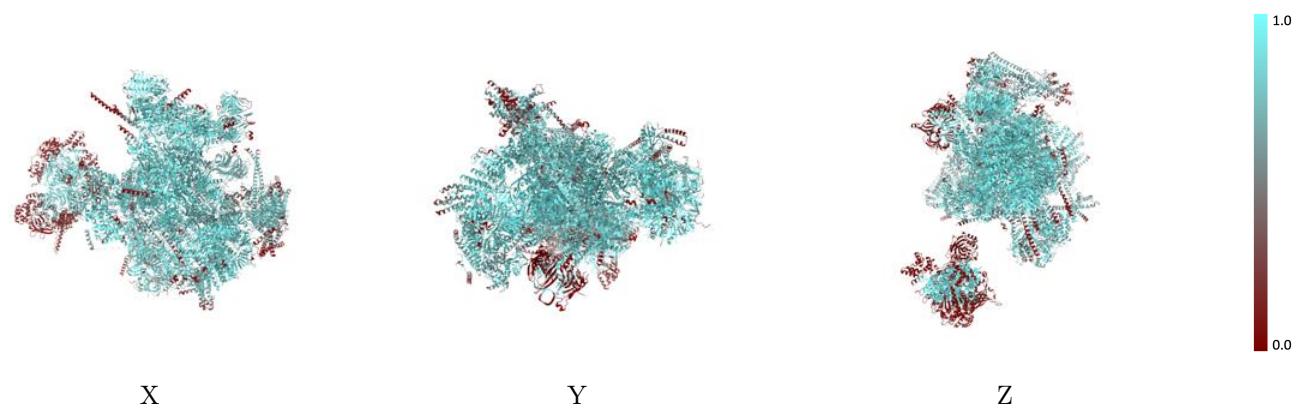
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



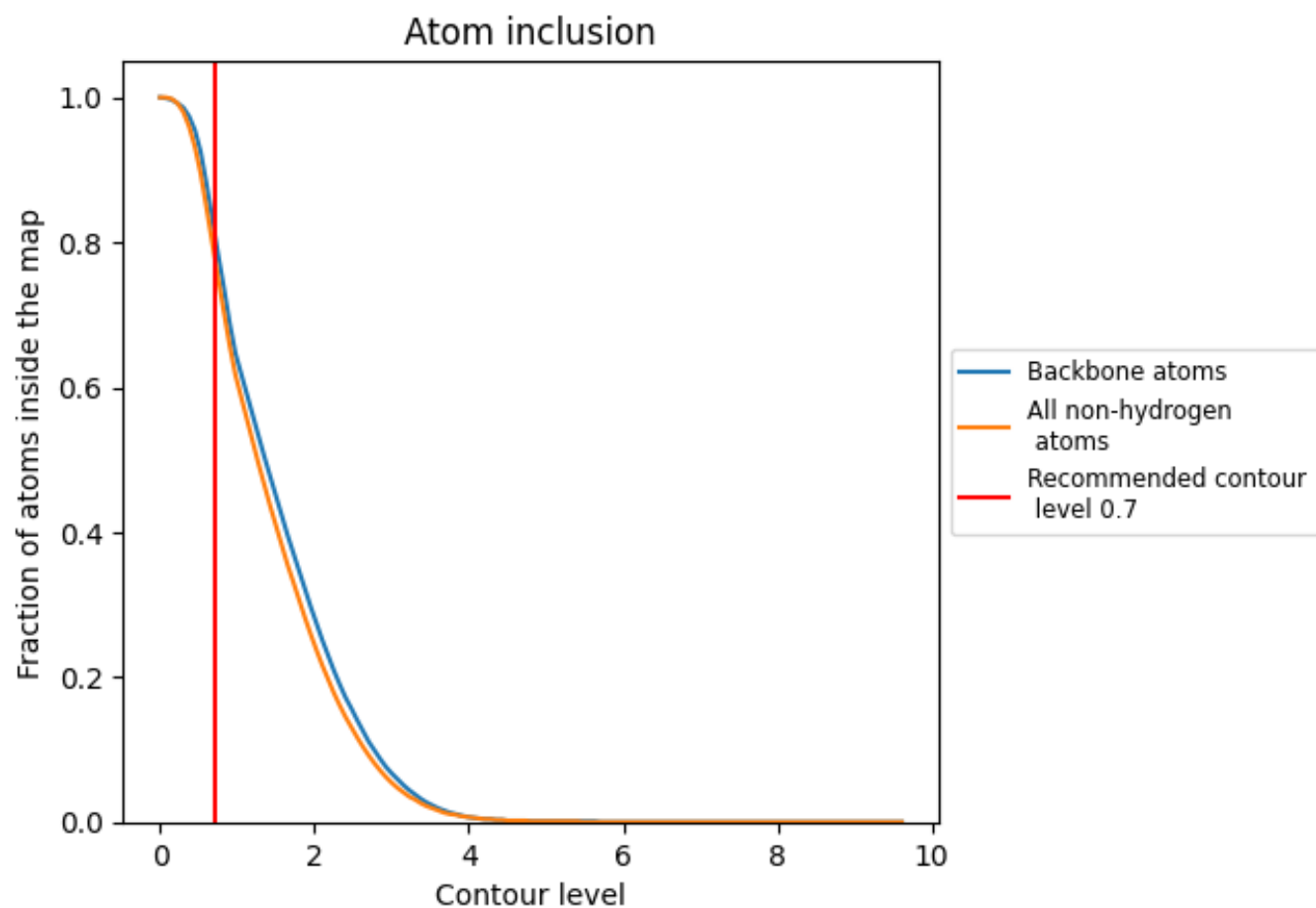
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.7).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7830	 0.4580
24	 0.7540	 0.4860
25	 0.7150	 0.4820
2C	 0.8230	 0.5380
2D	 0.9010	 0.5510
2H	 0.8170	 0.5070
2I	 0.7890	 0.5050
2J	 0.7640	 0.4970
51	 0.8350	 0.4900
52	 0.7560	 0.4640
53	 0.8270	 0.5050
5B	 0.7130	 0.4380
5E	 0.8060	 0.4840
5F	 0.8000	 0.5090
5G	 0.7520	 0.4760
62	 0.8120	 0.5130
63	 0.8690	 0.5350
64	 0.9000	 0.5580
65	 0.8960	 0.5410
66	 0.9100	 0.5590
67	 0.9090	 0.5600
68	 0.8900	 0.5570
L7	 0.9150	 0.5690
L8	 0.8100	 0.5250
L9	 0.8090	 0.5210
LA	 0.8820	 0.5640
LB	 0.4450	 0.0290
LC	 0.8750	 0.5250
LD	 0.6730	 0.4260
LE	 0.9310	 0.5860
LF	 0.8100	 0.4040
LG	 0.6350	 0.4710
LH	 0.6420	 0.4320
LJ	 0.9120	 0.6100
LL	 0.9310	 0.5760



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Chain	Atom inclusion	Q-score
LN	 0.8240	 0.4830
LO	 0.8490	 0.3110
LP	 0.8590	 0.5760
LQ	 0.7790	 0.5170
LR	 0.5800	 0.3850
LS	 0.8230	 0.4430
LT	 0.8490	 0.4830
LV	 0.7650	 0.3940
LW	 0.8250	 0.5450
LY	 0.8530	 0.5620
LZ	 0.7570	 0.4410
N2	 0.9080	 0.5460
N5	 0.9080	 0.5560
N6	 0.9420	 0.5700
RN	 0.8660	 0.4450
SA	 0.8800	 0.5560
SC	 0.8530	 0.5450
SD	 0.7760	 0.4920
SF	 0.5270	 0.4070
SJ	 0.8190	 0.4790
SK	 0.8380	 0.4460
SL	 0.7910	 0.5220
SN	 0.8670	 0.5530
SO	 0.8790	 0.5560
SP	 0.4290	 0.3090
SQ	 0.5990	 0.4310
SS	 0.7040	 0.4660
ST	 0.7120	 0.4850
SU	 0.6930	 0.4660
SV	 0.4610	 0.3280
SW	 0.6360	 0.4320
TN	 0.4650	 0.2660
U1	 0.3640	 0.0390
U2	 0.2700	 0.0130
U3	 0.3100	 0.0410
UB	 0.3670	 0.0520
UE	 0.3890	 0.0280
UF	 0.2720	 -0.0010
UG	 0.3980	 0.0220
UX	 0.6570	 0.3410